Development of a zeolite washcoating technique for microchannel reactors

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Lara Truter

Synopsis

Microreactor technology is becoming an increasingly active research field in terms of chemical reaction engineering and process intensification. An important feature of microreactor technology is the requirement of a catalyst layer. In the microchannel reactor configuration an alternative method is required to conventional reactors for incorporating catalysts whereby the catalyst is deposited onto the walls of the microchannels. The incorporation of zeolite catalysts into microchannel reactors can be done by either a direct synthesis method or a washcoating method. The zeolite washcoating method has been applied less frequently in microchannel reactors but is advantageous due to its simplicity and use of a pre-synthesised zeolite.

Using the Zapf et al. (2006) γ-Al_2O_3 washcoating method for microchannel reactors as a basis, the zeolite washcoating method was developed. Concepts from zeolite washcoating onto monoliths were additionally applied to improve the suspension and coating properties. Directly substituting the γ-Al_2O_3 powder used in the Zapf et al. (2006) washcoating method for a combination of 75% zeolite crystal agglomerate powder of reduced particle size (below 10 µm) and 25% γ-Al_2O_3 binder resulted in a minimal catalyst loss of 0.1% after adherence testing. A typical coating had a catalyst loading of 45 - 50 mg and coating thickness between 30 and 46 µm. The zeolite crystal size and structure was found to not be affected by any of the washcoating preparation steps.

A chemical reaction was additionally carried out in the microchannel reactor and fixed-bed reactor in order to further test the performance of the developed zeolite washcoating. The synthesis of the fine chemical, thymol, by the selective alkylation of *m*-cresol using isopropanol, was the chosen test reaction. The washcoating method resulted in an improved catalytic activity in comparison to the original zeolite crystal agglomerate powder. The substitution of Si framework atoms for Al contained in the alumina binder was thought to result in the formation of new acid sites and hence improved activity. The thymol selectivity of the respective catalysts was relatively comparable.

The microchannel reactor's conversion was found to be lower in comparison to the simulated washcoating in the fixed-bed reactor. Poor flow distribution in the microchannel reactor was thought to cause a lower conversion in the microchannel reactor resulting in a lower residence and higher actual WHSV.

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Glossary

Binder	additive with small particle size (organic or inorganic)
Dipping	immersion of monolith into washcoating suspension
Direct synthesis	zeolite grown directly onto substrate
Drop test	specific coating adherence test for the test plates
Metal sleeves	used for insulation of microchannel reactor
Microchannel reactor plate	microchannel plate with inlet and a outlet portals
Microchannel reactor	combination of coated microchannel reactor plates together to conduct a chemical reaction
Micro-structuring	formation of microchannels in plate
Microchannel sealing/bonding	joining of microchannel reactor plates to form microchannel reactor
Microsplitter	reagent flow splitter to obtain lower flow rates
Monolith	substrate which is coated with catalytic material
Phenolics	aromatic compounds consisting of a benzene ring substituted with a hydroxyl group
Simulated washcoating	ex-situ preparation of washcoating for application in fixed-bed reactor
Spalling	to break or chip off pieces of coating
Suspension/slurry	washcoating mixture containing the catalyst and other additives
Test plate	microchannel plate without inlet and outlet ports
Washcoating/ indirect synthesis	pre-synthesised catalyst and other additives are combined followed by coating onto the substrate

Nomenclature and symbols

Symbol	Description	Unit
BEA	zeolite β	
BET SA	BET surface area	$[m^2/g]$
CV	Control valve	
d_p	Particle diameter	[m]
Φ	Diameter	[m]
EDX	Energy-dispersive X-ray spectroscopy	
f_i	GC response factor of species i	
F	Filter or flow	
FIC	Flow indicator and controller	
FID	Flame ioniser detector	
γ	gamma	
GC	Gas chromatograph/gas chromatogram	
GCMS	Gas chromatograph mass spectrometry	
HPLC	High pressure liquid chromatography	
m	meta	
M	Metal	
MOR	Zeolite mordenite	
MFI	Zeolite ZSM-5	
MFC	Mass flow controller	
n	normal	
nm	nanometer	
NV	Needle valve	
p	para	
PEG	Polyethylene glycol	
P	Pressure	[bar]
PA_i	GC peak area of species i	$[m^2]$
PAC_i	Corrected peak area of species i	$[m^2]$
PAM_i	Mol proportional value of species i	$[m^2]$

Symbol	Description	Unit
PR	Pressure regulator	
PVA	Poly vinyl alcohol	
PI	Pressure Indicator	
$-r_a$"	Rate of reaction	[s^{-1}]
S	Selectivity	[mol %]
S	Microchannel reactor sleeve	
SEM	Scanning electron microscope/ microscopy	
SS	Stainless steel	
SRV	Safety relief valve	
T	Temperature	[^oC]
TI	Temperature indicator	
Tylose	Methylhydroxyethyl cellulose	
U	Overall heat transfer coefficient	[$kW/m^2.K$]
µ	Micrometer	
V	Valve	
VOC	Volatile Organic Compound (s)	
ŋ	Viscosity	[cP]
$ŋ_o$	Viscosity of pure suspension	[cP]
WHSV	Weight hourly space velocity	[$g_{m\text{-}cresol}/g_{zeolite}h$]
wt	Weight	
XRD	X-ray diffraction	
X	Conversion	[mol %]
Y	Yield	[mol %]
ζ	Zeta potential	[mV]

1. Introduction

In recent years, microchannel reactor technology has become an increasingly active research area due to several advantages gained over conventional reactor technology. These reactors have inner dimensions of tens to hundreds of micrometers which allow transport phenomena such as mass and heat transfer to be enhanced. Potential commercial applications of microchannel reactors have resulted in several companies such as IMM (Institut für Mikrotechnik Mainz), in Germany, and Velocys, in America, to be established over the last two decades. However, the commercial implementation of microchannel reactor technology to date is limited.

Microchannel reactors consist of a network of microchannels which allow the reactants and products to flow through. Catalysts are commonly used in microchannel reactors as is common to conventional chemical processing, however, in the case of microchannel reactors the catalyst is coated onto the microchannel walls. This has the advantage of achieving a higher productivity in comparison to conventional packed bed reactors, as well as ensuring that almost all of the catalyst is available for reaction at a fraction of the pressure drop occurring in conventional packed beds (Zhang et al., 2004). A coating technique is therefore an important prerequisite in order to incorporate the catalyst into the microchannel reactors.

The technologies currently available for coating catalysts onto microchannel reactor channel walls can be split with respect to two classes of catalysts: metal oxides and zeolites. Metal oxide catalyst coating techniques are well developed and understood. IMM for instance uses a washcoating technique which has particular application for fuel processing (Kolb et al., 2007). Zeolite catalyst coating techniques are however different. With zeolites, a washcoating technique (indirect synthesis) can be used or alternatively, a direct synthesis method which entails the zeolite being grown onto the microchannel walls may be applied. Zeolite H-ZSM-5 has been successfully coated onto stainless steel microchannels by direct synthesis, whilst the

less frequently applied washcoating method has only been used to coat silicon microchannel reactors and various monoliths.

The microchannel reactors currently being used for research purposes by Nelson Mandela Metropolitan University (NMMU) in South Africa have been both fabricated and coated with catalyst by IMM in Germany. Due to the catalyst layer influencing the reaction parameters significantly, it is desirable to be able to fabricate the microchannel reactors and coat the catalysts in South Africa. This will allow processes to be developed and optimised faster and more thoroughly, as well as allow South Africa to get up-to-date with current research trends.

The production of fine chemicals from local raw materials in South Africa is promising due to the higher market value obtainable from the workup of the raw materials and the resulting value addition. Manufacture of fine chemicals based on phenolics (aromatic compounds consisting of a benzene ring substituted with a hydroxyl group) is particularly attractive in South Africa because of the large quantity of such phenolics produced in the country. The phenolics are produced as a by-product by the Sasol synfuels refineries during the gasification of coal in Lurgi gasifiers.

In order to test the success of the catalyst coating technique developed in this study, various analytical tests were undertaken on the coated catalyst. A chemical reaction was also carried out in the microchannel reactor in order to further test the performance of the catalyst coating using this technique. The synthesis of the fine chemical thymol by the selective alkylation of *m*-cresol using isopropanol over a wall coated zeolite catalyst was studied. This reaction was chosen for reasons such as the availability of raw materials from South Africa's chemical industries, in particular phenolics, the production of fine chemicals in microchannel reactors to be one of the main potential industrial applications of microchannel reactors, and the experience with this reaction in the research group at the University of Cape Town.

2. Literature Review

2.1. Microchannel reactors

Microchannel reactors can be defined as a casing for performing reactions which results in micro-flow phenomena whereby characteristic flow guidance and unique processing properties occur (Hessel et al., 2005). Typically, a microchannel reactor consists of a network of micron-sized channels which are connected to reservoirs containing reactants and products. This network of channels is termed an element or plate. These plates can be stacked together as indicated in Figure 2.1 to form a microchannel reactor. Various units can also be added to this network of channels such as mixers, heat exchangers and separators to perform functions similar to large-scale operation.

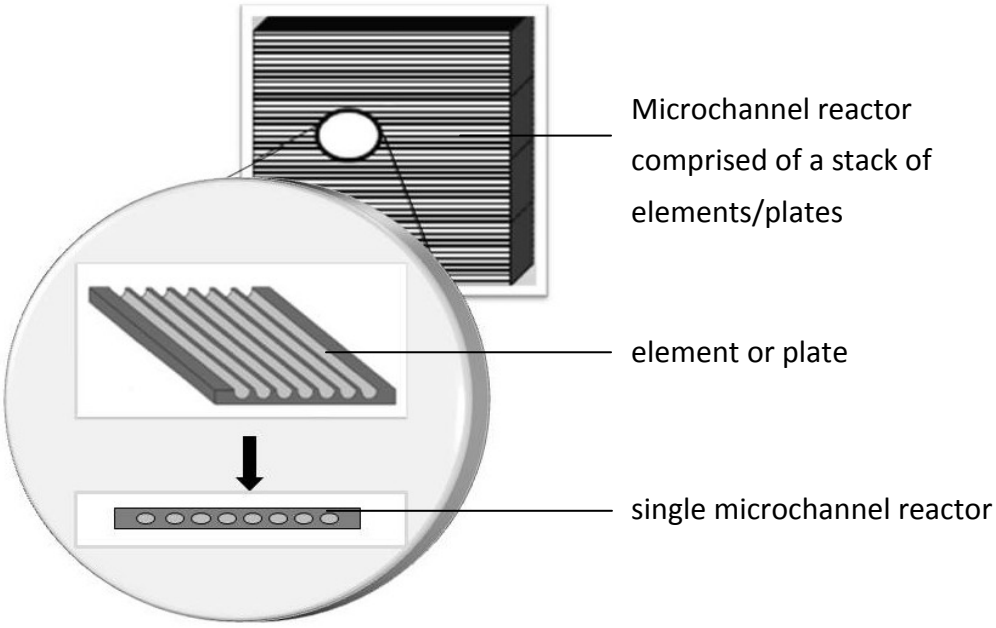

Figure 2.1: Basic configuration of a microchannel reactor (adapted from Hessel et al., 2005).
[The bottom of the enlarged image shows two coated microchannel plates sealed together face-to-face to form microchannels. These plates are then stacked together to form the microchannel reactor.]

2.1.1. Advantages and disadvantages of applying microchannel reactors

The advantages of microchannel reactors stem from the unique process intensification capabilities of these reactors in comparison to conventional reactors (Charpentier et al., 2007). One of the main aspects giving microchannel reactors superior performance when compared to conventional reactors is the increased surface-to-volume ratio (inverse of the hydraulic diameter) between 500 - 50 000 m^2/m^3 (Ehrfeld et al., 2000; Jähnisch et al., 2004; Mills et al., 2007). The advantages which stem from the high surface-to-volume ratios include superior mass and heat transfer properties, and improved hydrodynamic transport flow patterns in the microchannels. These unique properties allow for safe operation of highly exothermic reactions whilst preventing less deviation from optimal temperatures. Higher conversions and selectivities are also achievable in various reactions due to the higher residence time and lower mass transfer limitations (Wörtz et al., 2001). These individual advantages will be subsequently evaluated with regard to zeolites in the microchannel reactor configuration in Section 2.3.2.

Microchannel reactors have several advantages specific to either laboratory or industrial application. Laboratory applications benefit by microchannel reactors providing flexible reactor designs due to a parallel arrangement, quality experimental data which is accurate and detailed, and a large quantity of data being obtained faster and at lower costs (Hessel et al., 2004). Industrially, there is an incentive to reduce the amount of time when scaling up from laboratory to industrial scale. Microchannel reactor scale-up by simple stacking (numbering up) of several laboratory microchannel reactors avoids costly redesign and pilot-plant experiments, therefore shortening the development time from laboratory to industrial production.

The disadvantages of microchannel reactors in production stem from the scaling law whereby the processing equipment becomes more cost-effective with increasing size, based on the "sixth tenths factor law" (Peters, 2003). It can however be argued that the economy of scale in microchannel reactors is shifted to plant commissioning. A large number of smaller units are built instead, reducing the discrepancy between laboratory and plant operation (Hessel et al., 2005). Another significant challenge encountered when numbering up from an individual microchannel reactor to a multiple stack of microchannel reactors, is the ability to uniformly distribute the inlet flow to the parallel arrangement of microchannel reactors (Quiram et al., 2007; Bayer et al., 2005). Fouling and the need for cleaning of the equipment are other

disadvantages to be overcome in order for the microchannel reactors to be commercialized (Wörtz et al., 2001).

2.1.2. Commercial applications of microchannel reactors

The commercial application of microchannel reactors depends largely on the economic viability of the process and product and, thus, will not be appropriate for every process. There are, however, some specific processes which are particularly suited for industrial application. The production of high-value chemicals which are required in small quantities is a particularly attractive application. Fine chemicals are foreseen to be one of the first applications for microchannel reactors in industry according to an international market study, PAMIR [Potential and Applications of MIcroReaction technology] (Kiesewalter et al., 2002). The higher heat and mass transfer rates possible in microchannel reactors enable improved reaction yield and conversion. In addition, the ability to adjust operating conditions in a controlled manner facilitates higher reaction selectivities and thus product purity (Pennemann et al., 2004; Roberge et al., 2005; Gravidilis et al., 2002).

The commercial application of microchannel reactor technology is still limited but there are some examples within the area of fine chemicals which show promise. One such example is the production of 1 kg/hr of propylene oxide which has been successfully implemented in a pilot plant setup (Klemm et al., 2008). This microchannel reactor uses a titanium silicate-1 zeolite catalyst to convert propene and vapourised hydrogen peroxide to form propylene oxide.

Another application of microchannel reactors is the optimization and discovery of catalysts due to the high-throughput screening capabilities (Hessel et al., 2003). The ability to obtain kinetic data has also been demonstrated in microchannel reactors (Besser et al., 2003; Zech et al., 2000).

2.2. Fabrication of microchannel reactors

Microchannel reactors are assembled from coated microchannel plates that are stacked together face-to-face and bonded to form the microchannel reactor arrangement. There are various techniques for each step depending on the reagents and the operating conditions

involved in the reaction. The main techniques will be mentioned in this section and the most relevant steps given in more detail.

2.2.1. Material of construction

The material of construction must take into account temperature, corrosion and thermal properties (Brand et al., 2006). Various materials such as glass (McCreedy et al., 2001), silicon (Wan et al., 2001), stainless steel (Kolb et al., 2004), aluminium and copper (Kestenbaum et al., 2000) have been used to make microchannel reactor plates.

Stainless steel microchannel reactor plates have been used in numerous microchannel reactor applications due to their mechanical stability and robustness at high temperature (Ehrfeld et al., 2000). More specifically, iron-chrominum-aluminium alloys are a particularly advantageous material due to the formation of a surface oxide layer during thermal pretreatment (Srinivasan et al., 2003; Aartun et al., 2004; Zapf et al., 2003). This oxide layer improves the adherence of the catalyst coating and is discussed in more detail in Section 4.3.1.

2.2.2. Micro-structuring

A micro-structuring technique must be implemented to form the microchannels in the plate. There are numerous methods available such as micro-milling, electrodischarge machining, wet chemical etching, punching, embossing, laser micro-machining, and sintering (Hessel et al., 2005).

Wet chemical etching was applied for micro-structuring of the stainless steel plates used in this study. In wet chemical etching, a photo-resist is masked onto the plates and an etching solution such as iron chloride is applied. It has been used in various applications and allows a relatively wide range (100 µm - 600 µm) of channel depths to be produced (Hessel et al., 2005). However, the presence of chlorine in the etching solution has been reported to cause catalyst deactivation (Twigg et al., 1996). To reduce the chlorine content, various microchannel plate pretreatment methods were studied and it was found that plate calcination in air at 800 °C greatly reduced the chlorine content in the stainless steel microchannel plates (Zapf et al., 2003).

2.2.3. Catalyst coating

The microchannel reactor configuration requires a new method for incorporating the catalyst into the reactor. In conventional fixed-bed reactors, the catalyst is packed as a bed in the reactor, whereas in the case of the microchannel reactor, this approach cannot be applied due to the large pressure drop and poor flow distribution which would result in the small channels. The catalyst is thus incorporated into the microchannel reactor by depositing the catalyst onto the walls of the microchannels.

There are various coating techniques available which are dependant on the material of construction and the catalyst. Supported metal catalysts (e.g. Pd, Ni, Cu, Zn) can be incorporated directly by various methods such as washcoating, chemical vapour deposition, cathodic sputtering, sol-gel deposition, electrophoretic deposition etc. (Mielle et al., 2006). Alternatively, a metal oxide layer can first be deposited (i.e. Al_2O_3) and the active metal impregnated onto this layer (Zapf et al., 2006). To incorporate zeolites, a washcoating method can be used or a unique direct synthesis method whereby the zeolite is grown directly onto the microchannel walls (Rebrov et al., 2001) may be applied. A more extensive description of catalyst coating with particular emphasis on zeolites is provided in Section 2.3.3.

2.2.4. Microchannel plate sealing/ bonding

Once the catalyst has been coated onto the microchannel plates, two plates are sealed together face-to-face to form the microchannel reactor. The type of bonding technique must take into account the maximum temperature the catalyst can tolerate in order to avoid damage. Laser welding is advantageous since the amount of energy used to join the microchannel plates is low and limited to only the edges of the plates, in comparison to conventional welding. Other bonding techniques which can be applied to microchannel reactors include electron beam welding, diffusion bonding, brazing, and sintering (Hessel et al, 2005).

2.2.5. Flow distribution in microchannel reactors

The ability to evenly distribute the incoming fluid into the numerous microchannels is a common problem encountered in microchannel reactor processing (Quiram et al., 2007; Bayer et al., 2005; Hessel et al., 2004). Poor flow distribution will result in an unequal residence time

distribution and consequently different product distributions in the various microchannels. The approach to enabling adequate flow distribution across the various microchannels is reliant on the pressure drop in the microchannels. The flow distribution uniformity improves as the difference between the pressure drop in the microchannel bundle versus that in the inlet chamber increases (Hessel at al., 2004).

Various microchannel reactor designs have been applied in order to achieve uniform flow in the channels. Microchannel reactors which consist of a centre inlet connected to the various microchannels have been widely used in literature and, consequently, this type of reactor design was used in this study. A modeling study of the fluid dynamics of this configuration is shown in Figure 2.2 which depicts the fluid streamlines in the inlet chamber. The centre channels show a greater streamline density versus the outer channels and, hence, fluid flow. The inlet chamber also contains various recirculation zones. Futhermore, in the case of washcoated microchannels, the thickness of the washcoating is also an important factor influencing the flow distribution in the microchannel reactor (Cominos et al., 2003).

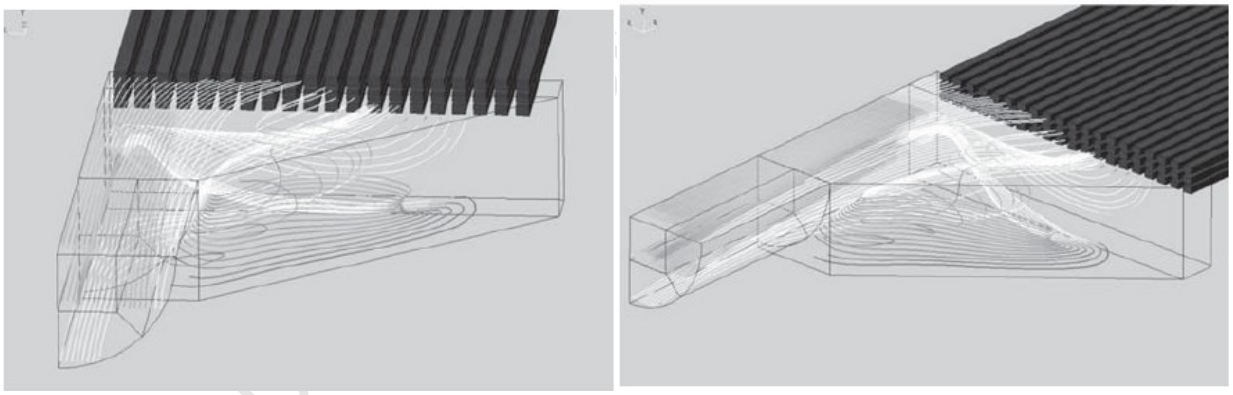

Figure 2.2: Flow streamlines in the inlet chamber of a microchannel reactor (Hessel et al., 2004).

2.3. Zeolite catalyst

Zeolites are crystalline alumina-silicates with regular pore systems having pore diameters in the range of 0.3 to 1 nm. The crystal framework consists of SiO_4^{4-} tetrahedra linked by oxygen bridges. Some of the Si^{4+} ions are substituted by Al^{3+} ions. The balancing charge can be a proton which creates a Bronsted acid site, forming an acid catalyst. The activity of the zeolite is a

consequence of its ability to act as a solid acid catalyst. A specific zeolite, H-MFI, was applied in this study for the reason of its known catalytic performance in phenolic transformation (Fletcher, 2003; van der Merwe, 2011; Nagooroo, 2011).

2.3.1. Properties of MFI zeolite

H-MFI is a medium pore zeolite in its acid- or H-form. H-MFI-90 is a generic material designation for a zeolite which is iso-structural with ZSM-5, is in its acid-form and which has a molar SiO_2/Al_2O_3 ratio of nominally 90; MFI being the structure-type designation of the International Zeolite Association (IZA).

The MFI framework forms two perpendicularly intersecting 10 membered-ring channels; a sinusoidal channel with almost circular openings of 0.54 x 0.56 nm diameter and a straight channel with an elliptical cross-section of 0.52 x 0.58 nm diameter. The sinusoidal channels connect two parallel layers of straight channels in a staggered way so that the pore system of the MFI zeolite is in fact also open for diffusion of molecules in the third dimension. (Santacesaria et al, 1990)

2.3.2. Zeolite catalysed reactions in microreaction technology

Zeolites, in general, have been implemented in various chemical and petrochemical processes, such as the production of fuels, synthesis of fine chemicals, pollution abatement, and as membranes (Coronas et al., 2004). As eluded to in Section 2.1.2, one of the applications of microreactor technology is seen to be in the production of fine chemicals. Zeolites show excellent potential for use in micro-scale applications due to their high selectivity (Coronas et al., 2004) and applicability to fine chemicals catalysis.

The overall performance of the microchannel reactor depends upon both the catalyst as well as the physical microchannel reactor configuration, such that a simultaneous optimization of both the catalyst coating technique and the microchannel reactor is preferred (Stefanescu et al., 2007). Reactions which will be particularly suitable in the microchannel reactor configuration are those which are fast, strongly exothermic/endothermic, complex, and multi-phase (Wörz et al., 2001; Lerou et al., 1996). Examples of such reactions are high temperature combustion and selective oxidations (Navascuès et al., 2010; Sebastian et al., 2009).

2.3.2.1. Internal mass transfer

In both the fixed-bed and the microchannel reactor, the internal mass transfer limitations are determined by pore diffusion in the catalyst. For the microchannel reactor, the reactants on the surface of the catalyst must diffuse through the catalyst coat to the channel wall. Similarly, in fixed-bed reactors, the reactants must diffuse through the catalyst pellets. For the microchannel reactor configuration, the catalyst layer is often much thinner in comparison to the pellet diameter which reduces the prevalence of internal mass transfer limitations (Walter et al., 2005).

Rebrov et al. (2001) compared a microchannel reactor to a Berty type reactor using the reduction of NO with ammonia as the test reaction. It was found that the reaction rate in the microchannel reactor (0.194 µmol NO/s.g_{cat}) was higher in comparison to the Berty reactor (0.144 µmol NO/s.g_{cat}). Internal mass transfer limitations in the pelletized catalyst used in the Berty reactor was thought to be the cause of the lower overall reaction rate. Similarly, Mies et al. (2007) found a higher activity in the microchannel reactor in comparison to the fixed-bed reactor due to the improved macropore diffusion in zeolite Beta coatings for the ammoxidation of ethylene to acetonitrile.

2.3.2.2. Heat Transfer

In the microchannel reactor configuration, overall heat transfer coefficients typically exceed 20 kW/m^2K which is greater than that of conventional heat exchangers which have overall heat transfer coefficients below 2 kW/m^2K (Ehrfeld et al., 2000). In several reactions the microchannel reactor achieved a higher conversion for the same temperature in comparison to the conventional reactor (Yueng et al., 2009; Sebastian et al., 2009; Navascuès et al., 2010). This was attributed to improved heat transfer in the microchannel reactor.

2.3.2.3. External Mass Transfer

In microchannel reactors, laminar flow prevails which makes external mass transfer only dependant on molecular diffusion driven by concentration gradients (Walter et al., 2005). The extent of the concentration gradient in the microchannels will mainly govern external mass transfer limitations in the microchannel reactor since there are no mixing effects as is found in the fixed-bed reactor. For the Knoevenagel reaction (between benzaldehyde and ethyl

cyanoacetate, ethyl acetate, and diethyl malonate), catalysed by Cs/NaX zeolite, the selectivity in the microchannel reactor was lower (78%) in comparison to the batch reactor (98%), a finding which was claimed to be a consequence of slower diffusion in the microchannel reactor channels which in turn permitted the bulky product molecules to further react to undesirable products (Yueng et al., 2009).

2.3.2.4. Conversion

As a consequence of the ability to use higher temperatures, higher conversions have been achieved in microchannel reactors in comparison to the conventional reactor counterpart. In the Knoevenagel condensation reaction of benzaldehyde, catalysed by Cs/NaX, a higher conversion of 38% was reported in comparison to the batch reactor (18%) (Yeung et al., 2009). Higher conversions in microchannel reactors were also reported for reactions catalysed by Pt/ZSM-5. The combustion of VOC and the selective oxidation of CO in the presence of H_2, CO_2, and H_2O resulted in near complete conversion (Navascuès et al., 2010; Sebastian et al., 2009).

2.3.3. Techniques for zeolite incorporation into microchannel reactors

The incorporation of zeolite catalysts into microchannel reactors can be achieved by two different coating techniques. In direct synthesis (hydrothermal synthesis), the zeolite is grown directly onto the substrate (i.e. the walls of the microchannels), whereas in indirect synthesis (washcoating) a pre-synthesised zeolite is prepared in a suspension which is coated onto the walls of the microchannels.

2.3.3.1. Zeolite direct synthesis

In direct synthesis, a one or two step process can be applied to form the zeolite coating. In the one step process, the seeding and growth of the layer occurs in the same step (Schoeman et al., 1997). In the two-step process, the seeding and growth steps are separate which is advantageous since these steps can be individually optimised (Rebrov et al., 2001). In the seeding step, the seeds are normally prepared separately followed by the attachment of the seeds to the surface by adsorption (Buciumen et al., 2001) or by grafting (Choi et al., 2005). Once the seeds have been attached, a dense layer of zeolite crystals is grown via hydrothermal synthesis.

2.3.3.2. Zeolite washcoating (Indirect synthesis)

Zeolite washcoating is a common method used to deposit zeolites onto monoliths whereas it is less prevelant for washcoating zeolites onto microchannel plates. A pre-synthesised zeolite powder is combined with various other additives to form the zeolite suspension which is coated onto the substrate, followed by drying and calcination.

2.3.3.3. Comparison of coating methods

Direct synthesis is the more commonly used method for coating zeolites onto microchannel plates. It is claimed to have the advantage of producing a more reproducible surface than washcoating, complete coverage of the walls (Jansen et al., 1998) and good adherence of the zeolite to the substrate (Wan et al., 2001). The layer can also be grown in specific locations such as in the microchannels only and not onto the bridges in between the channels (Wan et al., 2003). The direct synthesis method is however complex and requires a long synthesis time in comparison to the washcoating method, which has the additional advantage of being able to use a commercially available catalyst.

A comparative study of these two techniques was evaluated on silicon microchannel reactors using zeolites NaA, NH_4ZSM-5, and NaZSM-5 (Wan et al., 2001). The specific washcoating method applied used a commercial powder together with an undisclosed liquid and resulted in coatings which had a poor adherence and which were non-uniform (Figure 2.3 a & b). The direct synthesis method resulted in dense, uniform coatings with the zeolites having a specific crystal orientation. Figure 2.3c shows a coating with zeolite crystal orientation of <1 0 0> direction which exposes the zigzag pores to the surface. The <2 0 0> zeolite crystal orientated coating in Figure 2.3d, is the preferred orientation since this orientation gives molecules access to the interior set of pore channels. The thickness of the coating was also controllable by adjusting the seed population and hydrothermal conditions (Wan et al., 2001). Similar conclusions regarding the results from these two methods were reached when ZSM-5 was coated onto FeCrAlloy monoliths. In addition, the washcoating method gave a coating with randomly oriented zeolite crystals and additional mesoporosity due to the presence of additives in the suspension (Eleta et al., 2009).

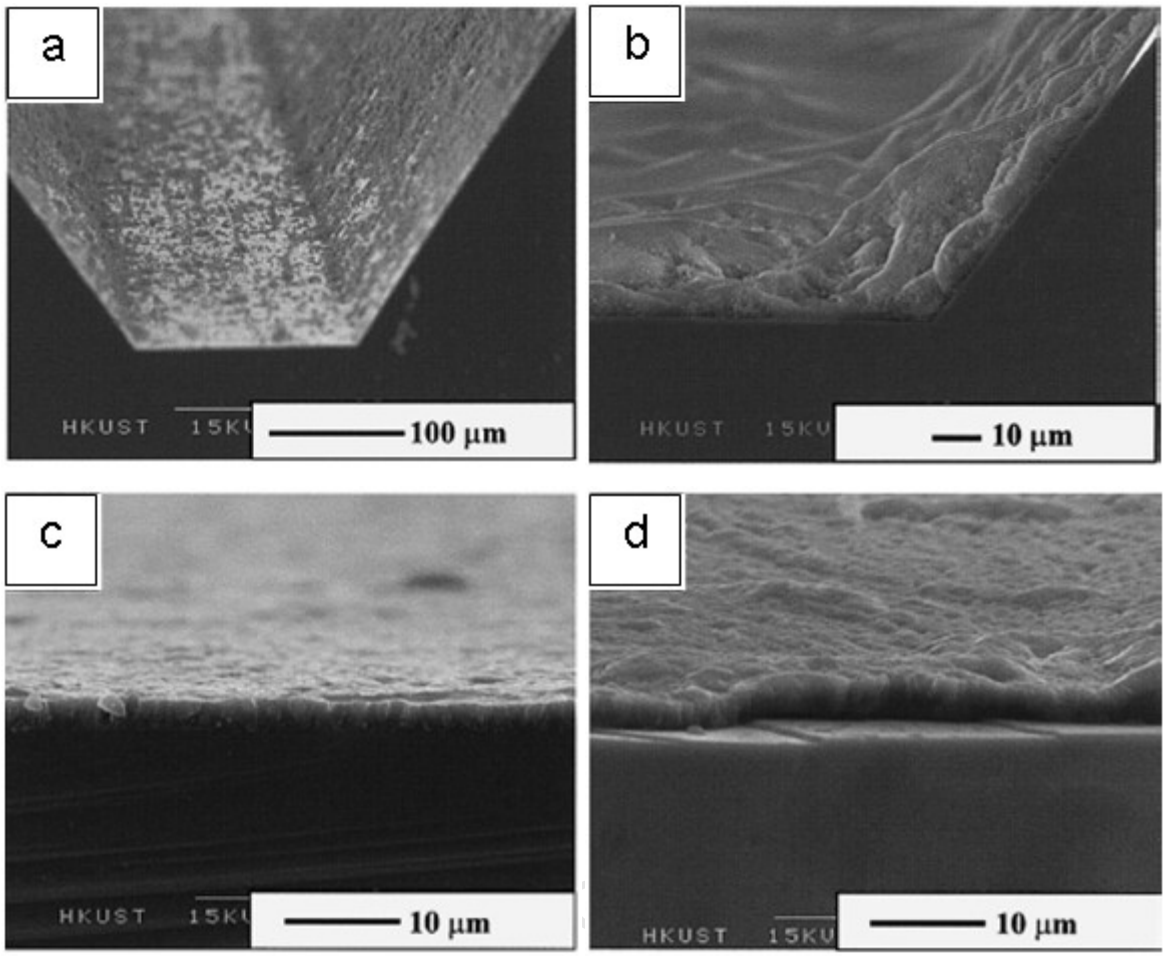

Figure 2.3: SEM images of various microchannel coatings. Washcoating: (a) NH_4ZSM-5, (b) NaZSM-5; Hydrothermal synthesis: (c), Si-1 coating <1 0 1> crystal orientation, (d) Si-1 <2 0 0> crystal orientation (Wan et al., 2001).

2.4. Washcoating fundamentals and technique

In washcoating, the nature of the support and the properties of the washcoating suspension are important factors which influence the final catalyst layer properties. The washcoating technique for coating zeolites has not yet been extensively used to coat microchannel reactors and not at all to coat stainless steel microchannel reactors. However, the zeolite washcoating technique has been successfully applied to monoliths made from various support material such as cordierite (Zamaro et al., 2005) and stainless steel (Eleta et al., 2009) which has resulted in catalytically active, well-adhering coatings. In terms of microchannel reactors, the washcoating technique described by Zapf et al. (2006) has frequently been applied to washcoat various metal oxides such as alumina, zirconia, ceria, and silica onto microchannel reactors. It is

therefore of interest to combine principles of monolithic zeolite washcoating and general microchannel reactor metal oxide washcoating, to develop a zeolite washcoating method for stainless steel microchannel reactors.

2.4.1. Differences between the microchannel reactor and monolith washcoating method

In monolith washcoating, the monolith is usually immersed in the suspension and removed from the suspension at a certain withdrawal velocity (termed "dipping"). Typically, the viscosity of the suspension will affect the amount of catalyst loaded since the excess will drip off. Blown air at a certain velocity is normally used to remove the excess suspension (Eleta et al., 2009; Nijhuis et al., 2001). In microchannel reactors, the microchannels are filled with the suspension, and the excess suspension is scraped off (Zapf et al., 2006).

The catalyst loading can be increased by re-dipping the monolith or, alternatively, using a higher viscosity suspension and solids concentration in the suspension (Valentini et al., 2001). With regard to microchannel reactors, the amount of suspension coated will depend on the microchannel dimensions and the solids concentration of the suspension. The drying and calcination steps in monoliths and microchannel reactors are relatively similar. Both are used to remove organic additives to result in the required layer formation.

Cordierite ($2MgO.2Al_2O_3.5SiO_2$) monoliths have been widely used as a substrate for the washcoating technique due to the high mechanical strength, low thermal expansion and good adhesion of the catalyst to the support. The macropores (3 - 5 µm) also allow for good anchorage of the particles (Agrafiotis et al., 1999). In contrast, fewer studies have been reported for washcoating on metal supports due to the smoother metal surface resulting in poorer adhesion of the catalyst layer (Eleta et al., 2009).

2.4.2. Rheology and other essential properties of the washcoating suspension

The properties of the washcoating suspension determine to a large extent the properties and quality of the final washcoated layer in the microchannels. The rheological properties of the

suspension, together with the general suspension composition, influence the state of dispersion of a powder in a suspension and hence the suspension stability (Vallar et al., 1999). Viscosity, zeta potential and pH are some of the variables which affect the rheology of the suspension and have been used in several studies to quantify the suspension stability (Vallar et al., 1999; Agrafiotis et al., 2000b; Nikolakis et al., 2005; Mitra et al., 2008).

2.4.2.1. Viscosity

The viscosity of the suspension influences the suspension stability, reproducibility and uniformity of the final catalyst layer, and is thus an important property to control in washcoating suspensions (Germani et al., 2007). The viscosity is dependant on various suspension parameters (i.e. particle size, solid concentration, suspension composition etc.).

A rheogram which plots viscosity versus shear rate gives the state of dispersion. A high viscosity which decreases with shear rate is known as pseudo-plastic or shear-thinning and results in suspensions which flocculate and do not disperse well. As the shear rate increases, the flocculants begin to break, increasing the degree of fluidity of the suspension. In contrast, viscosity that increases with shear rate, is known as dilatant or shear-thickening and leads to stable, deflocculated, and well dispersed suspensions (Vallar et al., 1999). Suspensions containing ZSM-5 zeolite, water and colloidal silica were reported to have a pseudo-plastic behavior (Mitra et al., 2008).

2.4.2.2. Zeta potential and pH

The suspension's zeta potential is an effective means for ascertaining the stability of the suspension and has been used in several studies for this purpose (Vallar et al., 1999; Agrafiotis et al., 2000b; Nikolakis et al., 2005; Mitra et al., 2008).

The zeta potential of a powder in suspension represents the extent of electrostatic repulsion between the particles. The surface charges of the particles determine the degree of dispersion and flocculation which will occur in a suspension. The isoelectric point is when the particles have no surface charge which results in flocculation to occur. At this point, the zeta potential is zero. As the absolute value zeta potential increases, the electrostatic repulsion of the particles increases which causes better dispersion of the particles and less flocculation. Figure 2.4 represents the zeta potential necessary for a stable suspension.

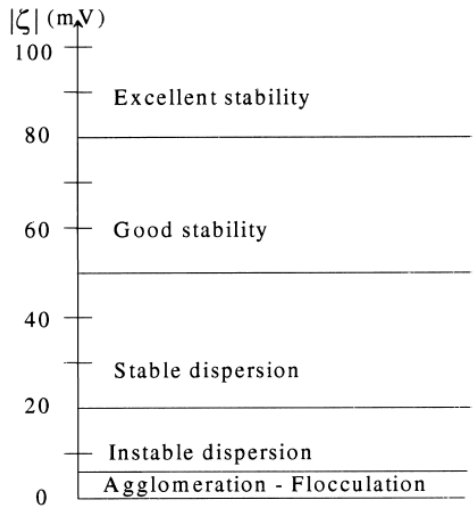

Figure 2.4: Slurry stability versus zeta potentials, ζ (Vallar et al., 1999).

The pH of the suspension influences the surface charge on the particles and thus the zeta potential. When dispersing a metal oxide powder in water, the pH influences the surface reactions of the metal oxide with water which forms M-OH species that dissociate to form acids and bases (Equation 2.1).

$M\text{-}OH_{surface} \Leftrightarrow M\text{-}O^-_{surface} + H^+$ in a basic suspension

$M\text{-}OH_{surface} + H^+ \Leftrightarrow M\text{-}OH_2^+{}_{surface}$ in an acidic suspension

Equation 2.1: Surface reactions of metal oxide compounds (Vallar et al., 1999).

The degree of dispersion is therefore influenced by the surface charges and hence zeta potential and pH. The zeta potential of zeolite ZSM-5 has negative values between a pH of 2 and 10 which results in well dispersed suspensions. No pH adjustment was therefore necessary (Mitra et al., 2008; Gopalakrishnan et al., 2007). In the case of other catalysts such as γ-Al_2O_3, the zeta potential passes through the isoelectric point at a pH of approximately 7.7 (Agrafiotis et al., 2000b) which is close to the pH of water and therefore requires the addition of an acid, base or deflocculant (Section 2.4.3.4) to ensure the suspension is stable. A detailed study of the effect pH has on the suspension properties found that, at a pH of 3.5, the adhesion of the final washcoat in stainless steel microchannel reactor channels is optimal for alumina suspensions (Peela et al., 2009).

2.4.3. Properties of the suspension

The basic components necessary for a washcoating suspension are the solid, which is desired to be deposited onto the support, and a solvent. There have also been a variety of additives such as binders, deflocculants, and acids used in the washcoating process. The effect of these components follows.

2.4.3.1. Solid concentration

The concentration of the solid is closely related to the viscosity of the suspension. Equation 2.2 gives a relationship between suspension viscosity and solid concentration.

$$\frac{\eta(\gamma)}{\eta_0} = \frac{1}{(1-\gamma)^{2.5}}$$

Equation 2.2*:* Relationship between suspension viscosity (ŋ) and solid concentration (γ).
[η_o is the viscosity of the solvent which in this case is pure water. The bulk density of the zeolite powder and the concentration of the suspension can be used to calculate the volume fraction of the solids. (Starov et al., 2002).]

Comparison of this equation to properties of a ZSM-5 suspension prepared by Zamaro et al. (2005) and Mitra et al. (2008) showed qualitatively similar results. Mitra et al. (2008) found the viscosity of the zeolite suspensions to increase exponentially with zeolite concentration (Figure 2.5) which corresponds to Equation 2.2. A practically logarithmic increase of viscosity is seen as long as the concentration does not exceed 50%. An increased solid concentration results in a lower interparticular distance and fluidity which causes the viscosity to increase. The variation of viscosity at a particular solid concentration for a certain zeolite (Figure 2.5b) can be attributed to different particle size distributions and morphologies of the zeolite powders (Mitra et al., 2008).

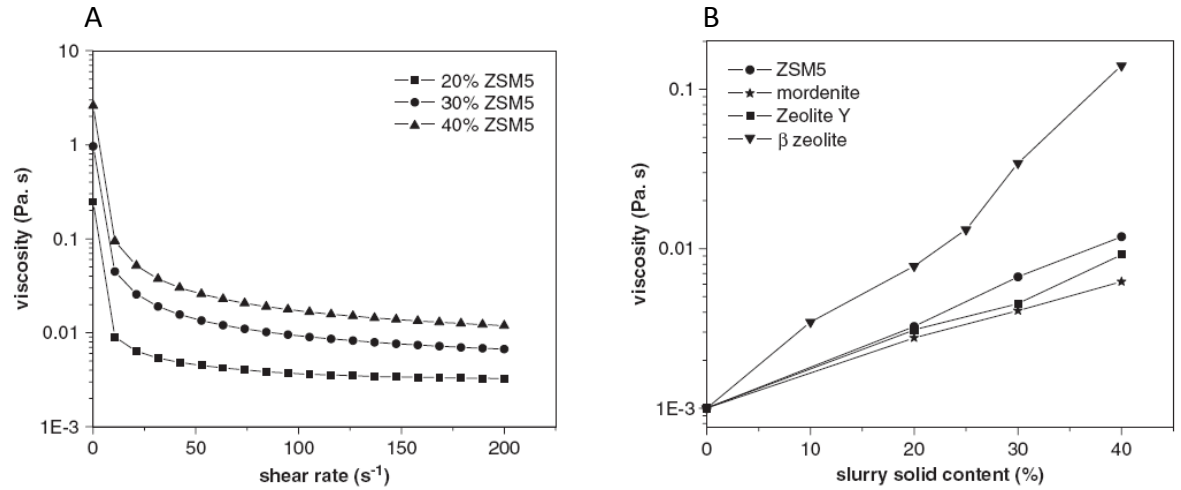

Figure 2.5: (A) Viscosity of ZSM-5 suspension at different solid concentrations; (B) Logarithmic increase of viscosities of different zeolite suspensions with solid content at a shear rate of 200 s^{-1} (Mitra et al., 2008).

The solid concentration is also an important variable affecting catalyst loading uniformity, reproducibility and adhesion of the final washcoat layer as described in Section 2.4.4.2.

2.4.3.2. Particle size

The particle size of the solid powder is an important variable in obtaining a stable suspension, and ultimately influences the properties of the washcoat layer.

Agrafiotis et al. (2000b) studied the effect of particle size (2 µm and 6 µm) on suspension properties such as viscosity, solid concentration, loading percentage and reproducibility for the washcoating of γ-Al_2O_3 onto cordierite monoliths. The larger particle's suspension viscosity increased almost linearly with solid content whilst the smaller particle's suspension viscosity increased exponentially. Suspensions containing smaller particles resulted in a larger suspension viscosity. Higher suspension viscosity increase catalyst loading for lower solid concentrations, requires fewer immersions and, thus, yields better reproducibility in comparison to the larger particles. No adhesion tests were done to compare the adhesion of washcoats from the two particle sizes applied in the study, however, in a previous study the adhesion of a washcoat from 2 µm particles was shown to produce a more adherent coating in comparison to washcoats from larger 17 µm and 52 µm particle sizes (Agrafiotis et al., 2000a).

Decreasing the particle size can, however, have detrimental effects on the zeolite crystal structure and thus influence the reaction conversion and selectivity. Dry ball milling of KNaX zeolites for 120 minutes was found to cause a collapse of the crystal structure but improved the selectivity of base catalysed reactions. (Xie et al., 1997). The particle size of the final zeolite agglomerates was not given, however, at long milling times it was thought that the individual zeolite crystallites were broken and thus of reduced crystallinity.

Wet ball milling of ZSM-5 powder reduced the particle size to 2 - 3 μm (Mitra et al., 2008). At low milling speeds and in the presence of water, any temperature rise which could cause the crystal structure to collapse was absorbed. The particle size of these zeolite agglomerates after milling is also larger than the size of the individual zeolite crystals therefore not affecting the crystallinity. The final particle size of the zeolite after milling should therefore exceed the size of the individual crystallites to avoid decreasing the intrinsic crystallinity. Subsequent washcoating of this reduced particle size zeolite onto a cordierite monolith improved the adherence significantly (Mitra et al., 2008).

2.4.3.3. Solvent

Apart from the convenience of using water as the solvent, the pH can easily be adjusted to form stable suspensions by the addition of an acid or base (Section 2.4.2.2). Water is used as the solvent in most washcoating suspensions. In principle, properties of the suspension can be modified using different solvents since the viscosity and surface tension of the solvent will affect the final washcoat layer. However, this has seldomly been implemented.

Butyl acetate was investigated, due to it having a lower surface tension, as an alternative solvent to water and was used to washcoat H-MFI onto cordierite monoliths. However, this resulted in a higher viscosity of the suspension and lower loading of the zeolite which was not favorable (Beers et al., 2003).

2.4.3.4. Deflocculant

The addition of deflocculants can help stabilise the suspension. Agrafiotis et al. (2000b) used NH_4-PMA (ammonium poly-methacrylate) as a deflocculant to obtain stable suspensions for coating γ-Al_2O_3 washcoats. The concentration of deflocculant required for stable suspensions at

a certain pH was determined from zeta potential data. The addition of the deflocculant also led to a lower suspension viscosity and improved the reproducibility of monolith catalyst loading.

2.4.3.5. Binder

A binder can be used to improve the stability of the suspension, as well as the adhesion and loading of the coating layer (Mitra et al., 2008). In general, there are two classes of binders: inorganic and organic. Typically, a binder consists of particles of a much smaller size than the solid which enables it to pack between the spaces of the larger catalyst particles. Organic binders improve the surface contact between the larger solid particles during the drying process but are ultimately removed during the calcination step. During the evaporation and calcination step, the small binder particles are carried to the points of contact between the larger particles due to capillary forces, so increasing the surface contact between the larger particles which aids in the anchorage of the catalyst particles (Agrafiotis et al., 2000a).

Poly vinyl alcohol (PVA) is a frequently used organic binder. The addition of PVA to a zeolite ZSM-5 suspension was found to improve the adherence of the washcoating onto FeCrAlloy monoliths (Eleta et al., 2009). In the methodology given by Zapf et al. (2006) for coating γ-Al_2O_3 onto microchannels, 5 wt% PVA was added to the washcoating suspension but no explanation for using this binder was given. However, Hwang et al. (2007) found, when coating alumina, that the addition of 1.5 wt% PVA resulted in a slower water evaporation rate during drying which prevented sudden shrinking and cracking of the alumina layer. To remove the PVA from the deposited layer, the Zapf et al. (2006) washcoating method suggests calcination at 600 °C. Temperature Programmed Desorption studies of Germani et al. (2007), showed that at 600 °C, under vacuum with no carrier gas, small amounts of PVA remained in the coating.

Poly vinyl alcohol (PVA), methylhydroxyethyl cellulose (Tylose), and polyethylene glycol (PEG) have been compared as organic binders for the alumina washcoating of microchannels (Germani et al., 2007). The binder's molecular weight and chemical structure influenced the thickening effect so that, for the same amount of binder, a trend of increasing viscosity was observed as: PEG < PVA < Tylose. Moreover, a higher bulk density coating resulted due to a greater shrinkage of the layer leading to cracking and thus poor adhesion. Tylose was found to provide the best compromise between layer density and shrinkage (Germani et al., 2007).

In terms of inorganic binders, colloidal silica has consistently been shown to improve the adhesion of ZSM-5 based zeolites to cordierite monoliths (Beers et al., 2003; Zamaro et al., 2005; Mitra et al., 2008; Eleta et al., 2009, Lisi et al., 2009). The addition of 6% colloidal silica was found also to improve the loading of ZSM-5 on FeCrAlloy monoliths (Eleta et al., 2009). Alumina has also been applied as a binder for the deposition of Cu-ZSM5 zeolite onto cordierite monolith but this resulted in poor adhesion (Lisi et al., 2009).

In addition to washcoating, silica and alumina have been used as a binder to produce zeolite extrudates. Typically, the binder is used to improve the mechanical strength of the zeolite extrudates, however, studies have shown the binder also to improve catalytic activity. The use of alumina as a binder has been shown to increase the intercrystalline (external) acidity of zeolites (Shihabi et al., 1985; Choudhary et al., 1997; Zhang et al., 2006). This additional acidity of the zeolite by alumina binder was thought to be caused by the formation of new acid sites (i.e. tetrahedral Al sites) due to the substitution of framework Si for the Al contained in the binder. To form these additional acid sites in the zeolite, Shihabi et al. (1985) describes a method whereby a ZSM-5 zeolite was steamed in the presence of a binder such as alumina to result in an increase in zeolite acidity and thus catalytic activity. The zeolite and alumina were initially mixed in the presence of water followed by drying. It should be noted that physical mixing does not result in an improvement in activity. For the conversion of *n*-hexane, the activity was found to increase whilst the selectivity remained constant in comparison to the original zeolite reaction results (Shihabi et al., 1985).

The effect of zeolite steaming in the presence of a binder also resulted in an improvement in catalytic activity for PtSnNa/ZSM-5 for the propane dehydrogenation reaction (Zhang et al., 2006) and ZSM-5 for the *n*-octane isomersization reaction (Lucas et al., 2004).

The presence of a binder can, however, cause detrimental effects to the catalyst. A non-stoichiometric spinel was formed when $Al(NO_3)_3$ binder was added to Co-ZSM-5 suspensions (Avila et al., 2005). Small surface area losses of the catalyst were observed when Tylose, PVA and PEG (Germani et al., 2007), and silica (Eleta et al., 2009) binders were used.

2.4.4. Properties of the catalyst washcoat layer

The catalytic performance of the final catalyst layer deposited onto the microchannels depends on the uniformity and reproducibility of the washcoat layer (since industrial applications need to use stacks of many microchannel reactors), the catalyst loading (thickness of the layer) and adhesion of the layer to the microchannel walls. Again, since only limited studies have reported on zeolite washcoating of microchannels in general, literature on the zeolite washcoat properties relates mostly to monoliths, whereas further information on microchannel washcoat properties must be derived from metal oxide systems.

2.4.4.1. Catalyst loading

Catalyst loading, in turn solid concentration and the number of washcoated layers, are the principle factors which determine the thickness of the washcoat layer. For the deposition of ZSM-5 washcoats onto cordierite monoliths, suspensions containing various zeolite concentrations were prepared and the number of immersions was varied (Zamaro et al., 2005). Figure 2.6 shows that increasing the solids concentration resulted in an exponential increase in zeolite loading, a finding which has been confirmed for alumina washcoats by Agrafiotis et al. (2000b). In the case of monolith coating, the viscosity will also affect the loading (Section 2.4.3.1). A higher solids concentration results in a higher viscosity and thus exponential increase in zeolite loading.

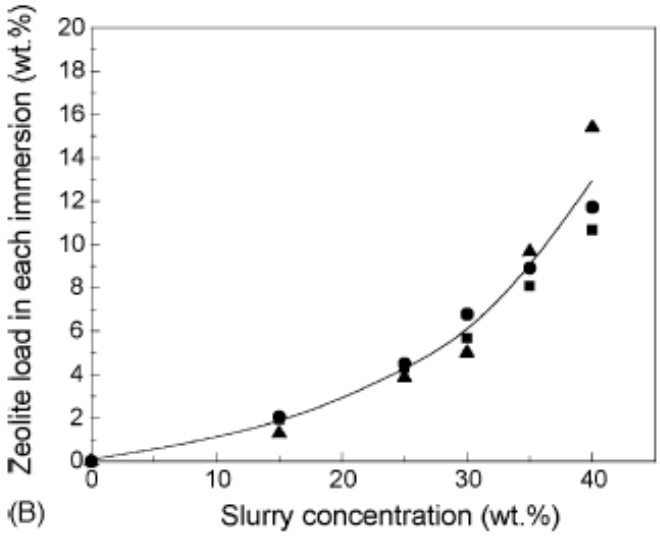

Figure 2.6: Effect of slurry concentration in monolith washcoating upon zeolite loading in the washcoat: (A) zeolite loaded in each immersion; (■) one immersion; (●) two immersions; (▲) three immersions (Zamaro et al., 2005).

Agrafiotis et al. (2000b) also found particle size to influence loading. For equal suspension viscosities, the larger particle (6 μm) suspension could accommodate a higher solids concentration than suspensions of 2 μm particles and therefore higher catalyst loading could be achieved with the larger particles. Alternatively, for suspensions with constant solid concentrations, the smaller particle (2 μm) coating resulted in a higher catalyst loading due to the higher suspension viscosity.

A high catalyst loading in the case of washcoating Cu-ZnO-Al_2O_3 catalyst onto silicon-based microchannel reactors resulted in layer cracking and spalling. This was overcome by decreasing the solids concentration (Hwang et al., 2007).

2.4.4.2. Uniformity and reproducibility

The uniformity and reproducibility of the catalyst layer should be high since large variations will impact on the other properties of the catalyst layer such as adhesion and catalyst loading, as well as reaction selectivity, conversion and mass transfer effects. It should be noted that even when very good homogenous coatings are obtained, a local non-homogeneity is present in each channel which is inevitable for the washcoating process (Avila et al., 2005).

Mitra et al. (2008) and Agrafiotis et al. (2000b) concluded (from washcoating monoliths) that a lower solids concentration (approximately 20%) should be used to enhance coating reproducibility. Mitra et al. (2008) found that the viscosity of the suspension influences the reproducibility and the uniformity of the catalyst layer. Low solids concentrations translate to a low viscosity suspension which improved both the uniformity and reproducibility of the coatings.

In terms of microchannel reactor coatings, viscosity was found to influence the coating uniformity as shown in schematic in Figure 2.7 (Germani et al., 2007). Once the microchannels have been filled with the washcoat suspension, drying and calcination proceeds whereby the organic compounds and water are removed to result in the final coating. Moreover, the viscosity of the washcoating suspension influences the uniformity of the final coating with high viscosity suspensions producing a thicker coating on the microchannel walls but with lower viscosity suspensions producing a thicker coating in the microchannel centre.

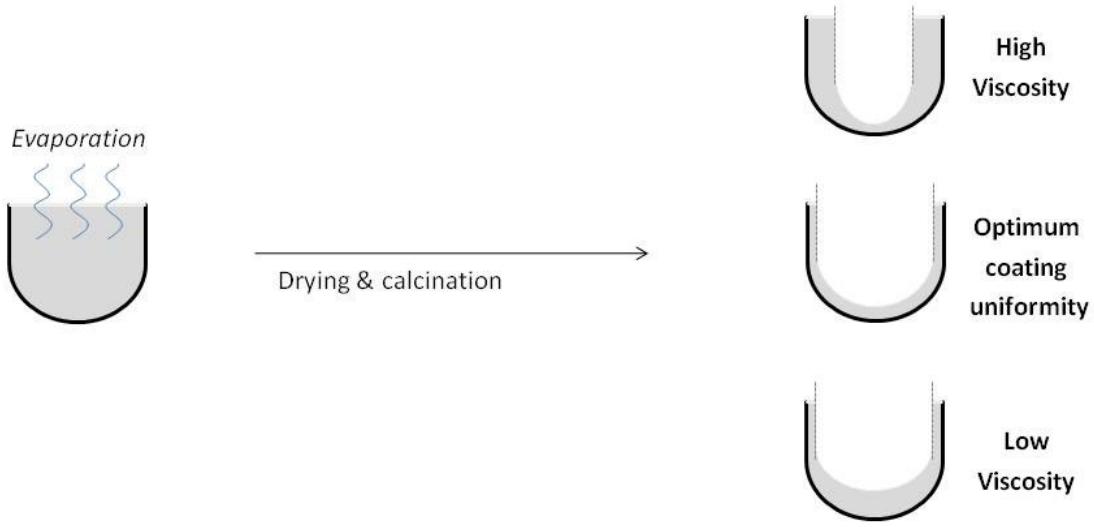

Figure 2.7: Influence of suspension viscosity on coating uniformity of microchannel reactor channels (Adapted from Germani et al., 2007).

2.4.4.3. Adhesion

One of the main limitations to the zeolite washcoating method in microchannel reactors is poor adhesion (Wan et al., 2001; Eleta et al., 2009).

To quantify the adhesion of a washcoat to the support, various adhesion tests have been devised. In one such method, the weight loss is recorded after exposing the coated support to ultrasonic treatment for 1 hour in petroleum ether and subsequent drying at 110 ˚C for 2 hours (Yasaki et al., 1993). This method has been used in studies on monoliths (Zamaro et al., 2005; Mitra et al., 2008) and microchannels (Germani et al., 2007).

A drop test has been developed to measure the adherence of coated microchannel plates (Zapf et al., 2006). In this test, the coated plate was dropped a fixed distance and the weight loss recorded. Figure 2.8 shows that no visible loss in γ-Al_2O_3 catalyst was seen after the drop test. A detailed description of these methods is given in the experimental Section 4.5.5.

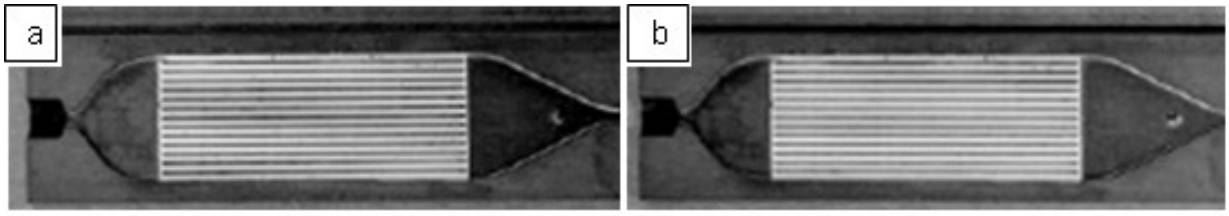

Figure 2.8: γ-Al_2O_3 coated microchannel reactor plates (a) before and (b) after drop test (Zapf et al., 2006).

For the adhesion of various oxide washcoats onto cordierite monoliths, the particle size was found to be the principal factor affecting the adhesion of the washcoat layer. Agrafiotis et al. (2000a) suggested that the adhesion of the coated layer to the support was attributed to a mechanical mechanism whereby the anchorage and interlocking of the particles to the support irregularities ensure adhesion. Similarly, decreasing the particle size of the zeolite suspension resulted in an improvement in adhesion for coating cordierite monoliths (Section 2.4.3.2).

Figure 2.9a shows the weight loss of zeolite washcoats after 1 hour ultrasonification as a function of particle size and solid concentration. Decreasing the particle size from 4 µm to 2 µm resulted in an improvement in coating adherence. Increasing the solid concentration decreases the adherence of the coating. The decrease in adherence with increasing solid concentration can be attributed to the increase in catalyst loading and the amount of catalyst loaded is dependant on the solids concentration. As the solid loading increases, the adherence decreases linearly (Figure 2.9b). The decrease in adherence with increasing zeolite concentration in Figure 2.9a is thus a consequence of the increased catalyst loading (Figure 2.9b).

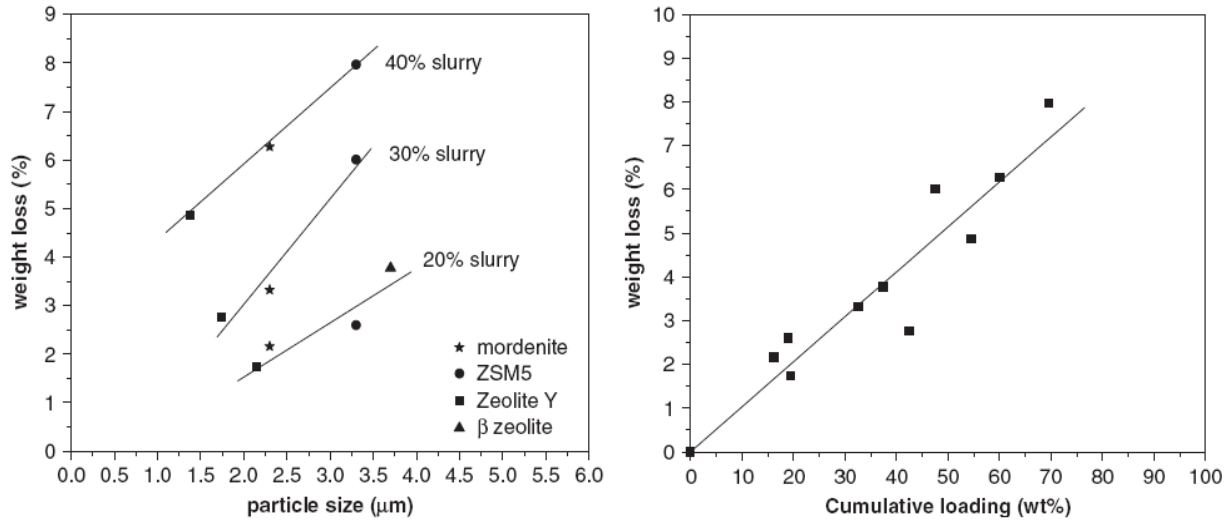

Figure 2.9: Weight loss of zeolite washcoats as a function of (a) particle size, slurry suspension and adherence weight loss (b) cumulative catalyst loading for particle size (2-3 μm) (Mitra et al., 2008).

As discussed in Section 2.4.3.5, the addition of a binder is another significant means to improve the washcoat adherence and has been implemented for zeolite washcoating onto monoliths (Beers et al., 2003; Zamaro et al., 2005; Mitra et al., 2008; Eleta et al., 2009; Lisi et al., 2009). The addition of a smaller particle binder has a similar affect to decreasing the catalyst particle size since the small particles of the binder increase the surface contact between the larger catalyst particles, thus providing better anchorage and inter-locking of particles (Section 2.4.3.5).

2.5. Fine chemical synthesis as test reaction

The overall performance of the microchannel reactor depends upon both the catalyst, as well as the physical microchannel reactor configuration. This requires the optimisation of both the catalyst coating technique, as well as the microchannel reactor to be done simultaneously. For this study, it was therefore essential that the developed zeolite washcoating technique be evaluated in the microchannel reactor configuration by conducting a chemical reaction to confirm the catalytic activity of the coating. Most of the reactions which have been considered for use in microchannel reactors have a high reaction rate and are highly exothermic (Section 2.3.2). However, in order to evaluate the catalytic activity of the washcoating, a slow reaction was chosen. The use of a slow reaction will allow any changes in conversion to be attributed to the activity of the catalyst and not other effects such as mass transfer.

The synthesis of the fine chemical, thymol, by the selective alkylation of *m*-cresol using isopropanol over a washcoated, H-MFI catalyst was the reaction considered. This reaction was additionally chosen due to it being a relatively well understood reaction as a consequence of previous work undertaken in the Centre for Catalysis Research at the University of Cape Town (Fletcher, 2003; Truter and Nagooroo, 2008; van der Merwe, 2011; Nagooroo, 2011).

2.5.1. Thymol applications

Thymol is a constituent of natural oils and also synthesised as a fine chemical which has applications as a fragrant, flavourant and intermediate in the perfume industry (Yadav et al., 2005). It can further be hydrogenated to menthol which is used as a flavourant and raw material for antiseptics, local anesthetic, antibacterial products and preservatives (Ashford, 1994). Approximately half of the thymol currently produced goes to the manufacture of menthol, which is a rapidly growing market (McCoy, 2010).

2.5.2. Industrial synthesis of thymol

The Bayer process is used for the industrial synthesis of thymol. The reagents, propene and *m*-cresol, react over an acid, activated alumina catalyst at operating conditions of 350 - 365 °C and 50 bar (Fiege, 2003). Small amounts of nitrogen bases such as ethanolamine are added. A 75% per pass conversion and selectivity of 80% is typically obtained (Fiege, 2003).

2.5.3. Alternatives for the synthesis of thymol

Although the yield of thymol obtained in the Bayer process is satisfactory, there are still some disadvantages such as the severe operating conditions, and the necessity to add nitrogen compounds. In this Section various alternatives to the industrial process are discussed.

2.5.3.1. Alkylating agent

The use of propene as an alkylating agent has the disadvantage of being gaseous at ambient temperature, making transportation, storage and handling difficult. The ability to produce propene in-situ via isopropanol dehydration can therefore be an attractive alternative. Van der Merwe (2011) studied various liquid alkylating agents as alternatives to propene (isopropanol,

n-propanol and diisopropyl ether) and found isopropanol to yield the best results in terms of selectivity and conversion.

2.5.3.2. Use of H-MFI catalysts for thymol synthesis

Various MFI zeolites have been applied to thymol synthesis, of which some studies are summarized in Table 2.1.

Table 2.1: Examples for synthesis of thymol from *m*-cresol using H-MFI catalysts.

Catalyst	SiO_2/Al_2O_3 ratio	Alkylating agent	T (˚C)	P (bar)	WHSV ($g_{feed}/g_{cat}h$)	Selectivity (%)	Conversion (%)	Reference
H-MFI	48	propene	250	2	3.5	75	34	(Wimmer et al., 1991)
H-MFI	90	propene	250	1	1.03	82	20	(Fletcher, J.V. et al., 2003)
H-MFI	90	*i*-propanol	250	15	0.4	68	52	(van der Merwe, 2011)
H-MFI	400	*i*-propanol	275	3	0.25	78	65	(Nagooroo, 2011)

2.5.4. Operating Conditions

The synthesis of thymol, alkylated by isopropanol and catalysed by H-MFI zeolites of different SiO_2/Al_2O_3 ratios was studied extensively by Nagooroo (2011). The results of the H-MFI-90 catalyst are summarised in Table 2.2. This same H-MFI-90 extrudate catalyst was used in this study.

Table 2.2: Thymol synthesis performance over H-MFI-90 zeolite (Nagooroo, 2011).

T (˚C)	P_{abs} (bar)	WHSV ($g_{feed}/g_{cat}h$)	$X_{m\text{-}cresol}$ (%)	S_{Thymol} (%)	Y_{Thymol} (%)
250	3	0.25	38	59	22
275	3	0.25	43	68	31
275	3	0.5	25	68	24

2.5.5. Reaction mechanism

Basically, two reactions dominate the acid catalysed isopropylation of *m*-cresol with isopropanol to synthesise thymol (6-isopropyl-3-methyl phenol), namely the very rapid dehydration of the isopropanol to propene followed by isopropylation of *m*-cresol with propene. The latter is shown in Figure 2.10.

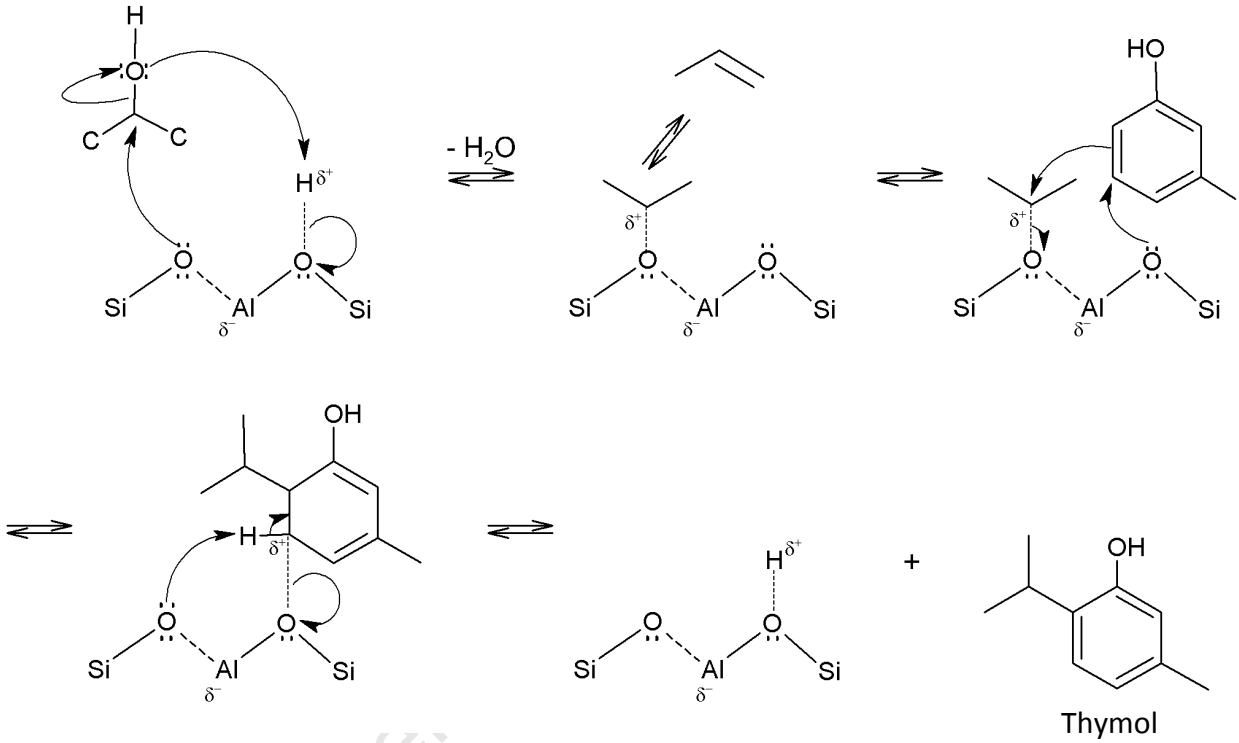

Figure 2.10: Reaction mechanism depicting the acid catalysed isopropylation of *m*-cresol with isopropanol (Truter and Nagooroo, 2008; Nagooroo, 2011).

The selectivity to thymol is higher by nature compared to the other isomers since thymol is the kinetically preferred isomer in the isopropylation reaction. The major by-products are isomers where the isopropyl group is in a different position on the phenol ring (Truter and Nagooroo, 2008; Nagooroo, 2011).

5-Isopropyl-3-methyl phenol (isomer with the isopropyl group substituted in the second meta-position) is the thermodynamically preferred isomer. The approximate equilibrium distribution of the thymol isomers is 20% thymol, 75% 5-isomer, 5% 4-isomer and an insignificant amount of the 2-isomer (Fletcher, 2003) as determined experimentally in the range of 250 ˚C - 350 ˚C.

The presence of thermodynamic limitations was found to occur with the propylation of *m*-cresol to thymol for reaction temperatures above 250 ˚C (Figure 2.11). For increasing reaction temperatures above 250 ˚C up to 350 ˚C, the thymol yield declined reflecting the exothermic nature of the propylation reaction of *m*-cresol to thymol.

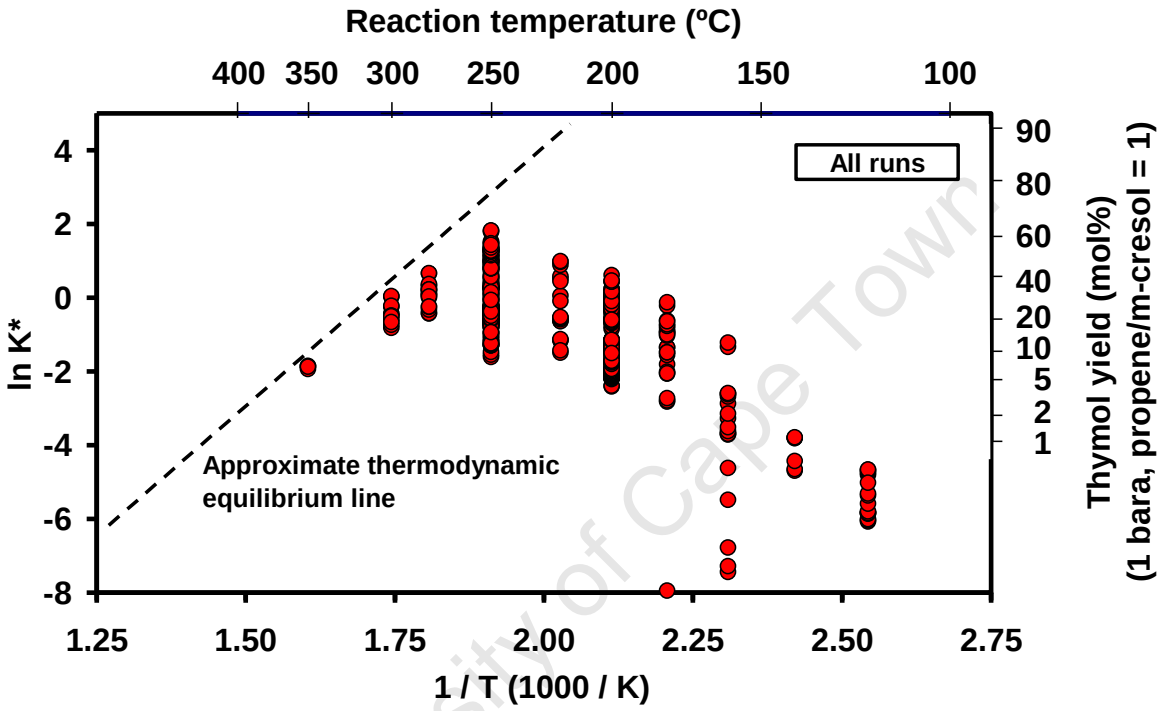

Figure 2.11: Thermodynamic equilibrium limitation for thymol synthesis from m-cresol and propene (Fletcher et al., 2001).

2.6. Summary of Literature Review

Microchannel reactors have unique properties in comparison to the conventional reactors. The smaller dimensions result in higher surface-to-volume ratios and improved transport properties in comparison to conventional reactors. For the inclusion of catalyst into the microchannel reactor, the catalyst must be coated onto the microchannel walls. Whereas, a washcoating method developed by Zapf et al. (2006) has been described to give adherent γ-Al_2O_3 coatings in microchannel reactors, zeolites have mainly been coated onto microchannels by the direct synthesis method and only limited literature has been reported using the washcoating method. Washcoating has the advantage of using a pre-synthesised catalyst including the ability to use different commercially available zeolites without having to change the coating methodology significantly, as well as allow for a more comparable evaluation of the microchannel reactor configuration to the conventional fixed-bed reactor.

Previous use of the zeolite washcoating technique in microreactors has resulted in poorly adhering, non-uniform coatings. The particle size of the zeolite has been found to be an important variable affecting the washcoat adherence whereby decreasing the particle size of the zeolite improves zeolite adherence onto monoliths. The addition of organic and inorganic binders is another effective means to improving coating adherence. The addition of an organic binder such as PVA improved the coating adherence and prevented sudden shrinking and cracking of the layer. Inorganic binders such as silica have also been shown to improve coating adherence in zeolite monolithic washcoats. The addition of γ-Al_2O_3 binder to zeolites has been found to increase zeolite acidity and thus activity when initially mixed together in water as is done in the washcoating method.

The uniformity and reproducibility of the washcoat is largely dependant on the rheological properties. Lower suspension viscosities result in a more reproducible washcoat, whilst the coating uniformity in microreactors is dependant on suspension viscosity. The solids concentration will determine the thickness of the washcoat layer and thus catalyst loading. Low solids concentration suspensions have shown to be most effective in terms of improving reproducibility and adherence.

The application of zeolites in microchannel reactors is interesting due to the high selectivity obtainable and relevance of microchannel reactors in the fine chemicals industry. The

production of fine chemicals in the microchannel reactor configuration is said to be one of the main potential applications of microchannel reactors with numerous fine chemical reactions being catalysed by zeolites. Typically, highly exothermic and high reaction rate reactions are used in microchannel reactors.

The production of the fine chemical, thymol, will be used as the reaction to test the activity and adherence of the zeolite washcoating, as well as compare the microchannel reactor to the fixed-bed configuration. Optimal operating conditions obtained in the fixed-bed reactor configuration were found to produce a 31% thymol yield for H-MFI-90 extrudates when using isopropanol as the *m*-cresol alkylating agent.

3. Objectives of study

3.1. Aim

The primary aim of this study was to develop a method to coat stainless steel microchannel reactor channel walls with a high silica H-MFI zeolite by adapting the Zapf et al. (2006) γ-Al_2O_3 washcoating technique to washcoat zeolite crystal agglomerate powder.

3.2. Objectives

1. To find out whether the washcoating method developed by Zapf et al. (2006) to deposit γ-Al_2O_3 catalyst onto microchannel reactor channel walls can be extended to coating high silica H-MFI zeolite crystal agglomerates onto the walls of stainless steel microchannel reactors by substituting the γ-Al_2O_3 powder for zeolite crystal agglomerate powder.
2. To determine and optimize the variables which result in a stable zeolite washcoating suspension.
3. To obtain a catalyst layer which has a good adherence to stainless steel microchannels, is uniform, reproducible, and has high catalyst loading.
4. To maintain similar catalytic properties to the original zeolite crystal agglomerate powder after washcoating as when applied in conventional fixed-bed reactor configuration.
5. To obtain a semi-quantitative comparison between catalyst performance in fixed-bed versus microchannel reactor configurations.

3.3. Hypothesis

Zeolite particle size and binder addition are the principal variables affecting washcoat physical properties, and suitable manipulation of these variables will result in a stable, uniform, and adherent catalyst layer with performance similar to conventional zeolite catalysts.

3.4. Key Questions

1. Can the washcoating method developed by Zapf et al. (2006) to deposit γ-Al_2O_3 catalyst onto microchannel reactor channel walls be extended to coating high silica H-MFI zeolite crystal agglomerates onto the microchannel reactor walls by substituting γ- Al_2O_3 powder for zeolite powder and adapting the coating parameters?
2. What are the main variables which need to be optimised to result in a stable zeolite suspension and what is the optimised set of variables?
3. What are the main variables which affect the properties of the resulting zeolite layer and what is the optimal set of variables?
4. Does the washcoated zeolite catalyst have different catalytic properties to the original H-MFI-90 zeolite powder?

4. Experimental

4.1. Raw materials and chemicals

4.1.1. Catalyst

The H-MFI-90 samples used were standard industrial materials from Süd-Chemie. The microchannel reactor washcoating experiments were conducted using H-MFI-90 powder, whilst in the fixed-bed reactor tests, H-MFI-90 catalyst extrudates were applied (Table 4.1).

Table 4.1: H-MFI-90 zeolite catalysts (Süd-Chemie).

Material Form	Particle Size	Zeolite content (%)	Crystallite size (µm)[e]	Nominal zeolite SiO_2/Al_2O_3 ratio (molar)
Powder[a]	34 µm[b]	100	< 0.1	90
Extrudates[c]	1/16''	80[d]	< 0.1	90

[a] *Agglomerates of small zeolite crystallites*

[b] *Average diameter of agglomerates (determined by Malvern microsizer)*

[c] *Extrudates of powder[a] and Al_2O_3 binder*

[d] *Nominally 20 wt% Al_2O_3 binder*

[e] *Nominal average zeolite crystallite size (Nagooroo, 2011)*

4.1.1.1. Pelletizing H-MFI-90 powder

To compare the activity of the two H-MFI-90 catalysts in the fixed-bed configuration, the crystallite agglomerate powder was pelletised, granulated and sieved to provide a 250 - 500 µm granulate sample. This was achieved by pressing the powder into tablets (approximately 2 g

powder per time). Once several tablets had been made, the tablets were lightly ground using a mortar and pestle and then sieved to produce a 250 – 500 µm fraction. Particles greater than 500 µm were again lightly ground and re-sieved. Particles smaller than 250 µm were discarded.

4.1.1.2. Reducing H-MFI-90 powder particle size

The particle size of the H-MFI-90 powder was reduced by breaking the crystal agglomerates into smaller fragments by use of a micronising mill. 5 g of zeolite powder and 10 ml of isopropanol were added to the milling container containing 16 ceramic beads. The powder was milled for 0-12 minutes to obtain different average particle sizes. The milling procedure was repeated until enough milled zeolite powder was obtained to prepare a batch of washcoating suspension. The milled powder, entrained with isopropanol, was dried at 120 ˚C overnight. A subsequent 600 ˚C calcination step (Figure 4.8) was found to be necessary due to the formation of carbon deposits on the zeolite as described in Section 5.2.1.2.

4.1.2. Washcoating suspension additives

The specifications of the additives used to prepare the washcoating suspension are given in Table 4.2

Table 4.2: Specifications of washcoating suspension additives

Type Material	Material Form	Mean Size	Manufacturer	Sample Code
γ-Al_2O_3	powder	3 µm	Alfa Aesar	CAS: 1344-28-1
Colloidal silica	40% suspension in water	n/a	Ludox	AS-40
Poly vinyl alcohol	beads	n/a	Fluka	40-88
Glacial acetic acid	liquid	n/a	Merck	-

4.1.3. Test reaction feedstocks

The reagents used were isopropanol (Merck) and *m*-cresol (Merisol). GC analyses of the isopropanol found no significant impurities to be present. The *m*-cresol contained some impurities, as indicated in Table 4.3.

Table 4.3: Impurity content in *m*-cresol feed (Merisol, >98%).

Component	Molar composition (%)
Isopropyl-Tolyl Ether	0.03
Phenol	0.04
o-Cresol	0.07
p-Cresol	0.63
m-Cresol	99.13
2,4-Xylenol	0.05
2,5-Xylenol	0.01
2,3-Xylenol	0.04

4.2. Microchannel plates

The microchannel reactor plates were obtained from Ätzetechnik Herz GmbH in Germany and were made from stainless steel 1.4571 with the elemental composition of the alloying elements given in Table 4.4. The microchannels were formed by wet chemical etching using an aqueous solution of iron trichloride (Section 2.2.2). Figure 4.1 shows a cross-sectional view of a microchannel before coating.

Table 4.4: Stainless steel microchannel plate composition (alloying elements).

Element	Elemental Wt %
C	≤ 0.08
Si	≤ 1.0
Mn	≤ 2.0
P	≤ 0.045
S	≤ 0.015
Cr	16.5 – 18.5
Mo	2.0 – 2.5
Ni	10.5 – 13.5
Ti	5 x C ≤ 0.70

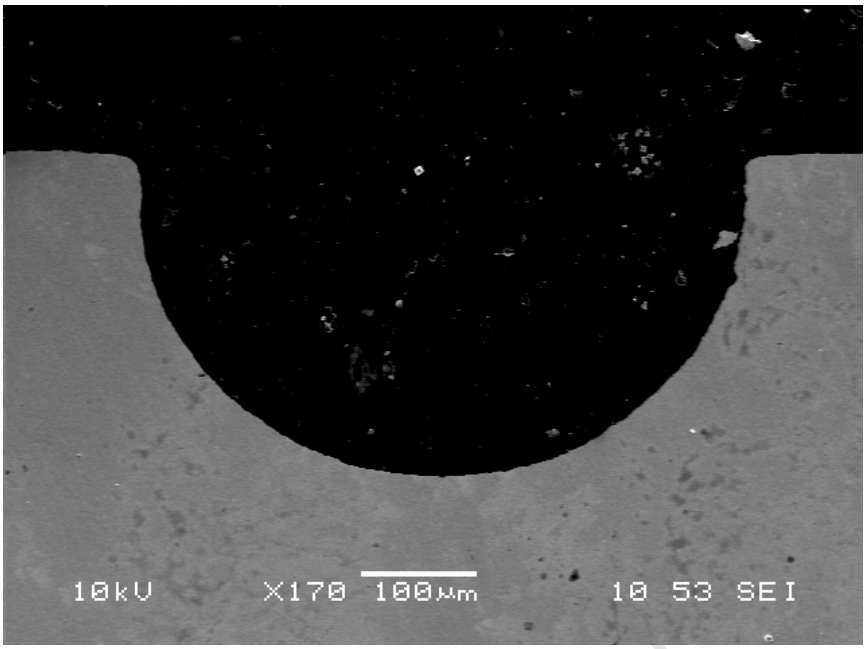

Figure 4.1: Stainless steel microchannel plate formed by chemical etching with iron chloride (cross-section).

A schematic view of a typical microchannel reactor plate is shown in Figure 4.2a with relevant dimensions provided in Table 4.5. In order for the microchannel reactor to be connected to the rest of the experimental setup, a 1/8" hole was required be made at the inlet and outlet of the microchannel reactor to incorporate a 1/8" tube. Two microchannel reactor plates were clamped together and a hole (1/8" wide) was drilled into the centre of the inlet and outlet ports to result in the corresponding holes as shown in Figure 4.2. Once these holes had been made, the plates could be pretreated and coated.

Test plates for development of the coating procedure differed from the microchannel plates in that they were designed for maximum microchannel coverage and were thinner material so as to minimize weight. These are presented schematically in Figure 4.2b with characteristic dimensions presented in Table 4.5 for five different test plate configurations, A to E. Unless otherwise stated, all coating development was carried out using test plate B which comprises of the same key channel dimensions as the microchannel reactor test plate.

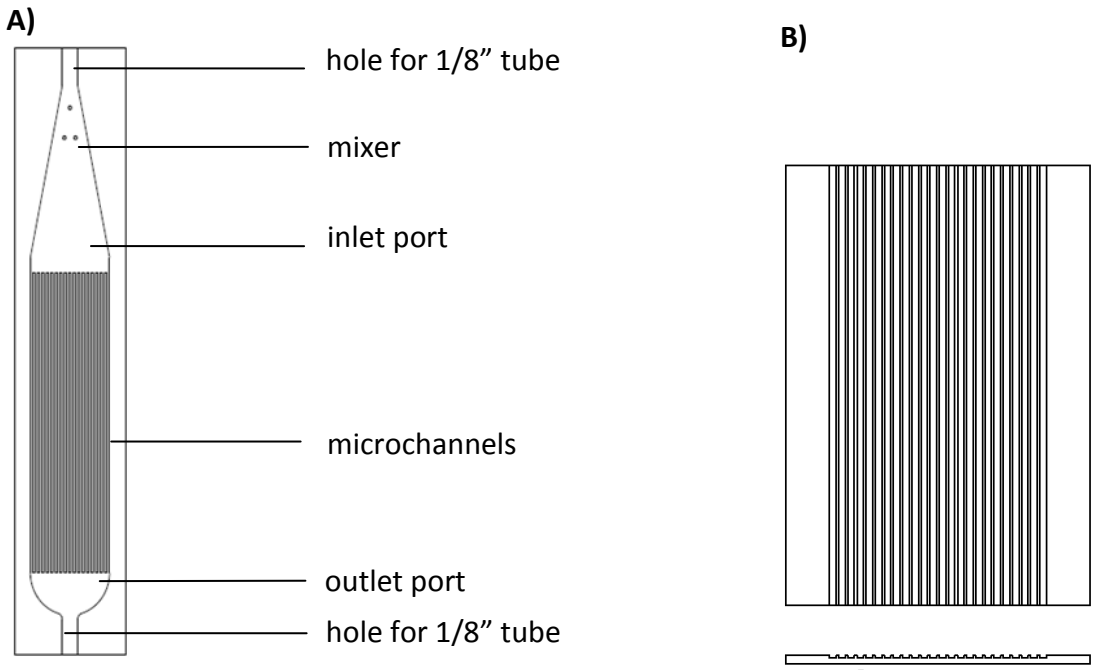

Figure 4.2: Example of a (a) microchannel reactor plate and (b) coating test plate (viewed from the top and lengthwise).

Table 4.5: Dimensions of microchannel reactor and coating test plates (mm).

Plate	Microchannel reactor	A	B*	C	D	E
Channel Width	0.5	0.35	0.5	0.75	0.4	0.5
Channel Depth	0.3	0.25	0.3	0.3	0.25	0.25
Bridge width	0.3	0.3	0.3	0.3	0.3	0.3
Plate length	40	50	50	50	50	50
Plate width	12	24.4	25.3	24.9	24.9	25.3
Plate Side width	2.15	5.3	4.85	5.05	5.05	4.85
No. of channels	15	38	32	24	36	32
Total width	16	35	35	35	35	35
Inlet length	30					
Outlet length	11					

* *Test plate B was used to evaluate the coating properties unless specifically stated otherwise.*

4.3. Washcoating methodology

The washcoating method used to coat the zeolite onto the microchannel plates was based on that for washcoating γ-Al_2O_3 by IMM (Zapf et al., 2006).

4.3.1. Pretreatment of plates

Before coating, the plates were cleaned and thermally pretreated in order to remove chlorine left from the etching process (Section 4.2) and to improve the adhesion of the subsequent catalyst washcoat. Cleaning involved treating with isopropanol in an ultrasonic bath for 10 minutes followed by drying in a fume cupboard at ambient conditions.

Subsequently, the plates were calcined in air at 800 ˚C for 2 hours according to the temperature programme presented in Figure 4.3. During calcination a metal oxide layer of similar properties to the washcoat and which improves adherence of the subsequent coating forms on the surface of the stainless steel plates (Zapf et al., 2006). After the thermal treatment, the plates lose their metallic luster and have a darker colour due to the formation of the metal oxide layer.

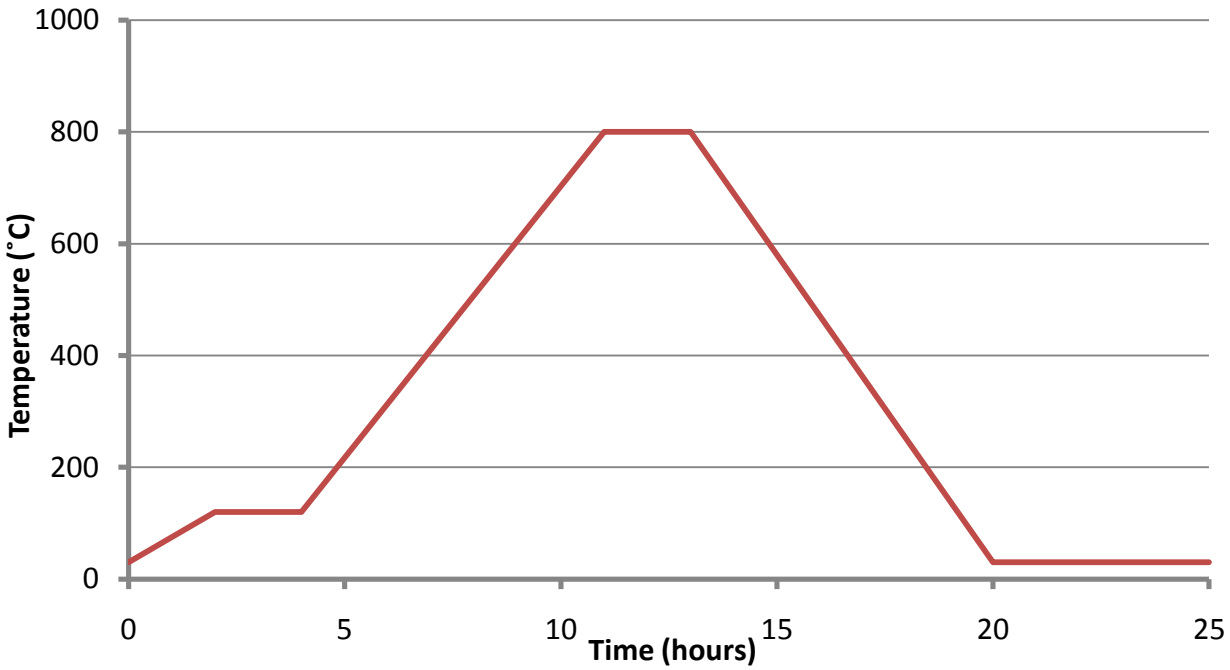

Figure 4.3: Temperature programme for the microchannel plate thermal treatment (holding temperatures at 120˚C and 800˚C for 2 hours).

In order to identify the plates, the plate number was engraved on the back of each plate after thermal pretreatment. Thereafter, the plates were weighed to the fourth decimal place. It should be noted that once calcined, the plates were not be handled without the use of gloves as a precaution against mass changes resulting from contact with bare hands.

4.3.2. Washcoat suspension synthesis

The washcoating suspension is synthesised using the general methodology described by Zapf et al. (2006) and Table 4.6 shows the typical composition of a washcoating suspension. In order to incorporate the zeolite catalyst, the γ-Al_2O_3 of Zapf et al. (2006) was substituted by the zeolite agglomerate powder in various percentages. The percentages of the other additives in the washcoating suspension, such as distilled water, polyvinyl alcohol, and acetic acid, were not altered unless explicitly stated.

Table 4.6: Typical washcoating suspension composition (for details of ingredients see Table 4.1 and Table 4.2).

Compound	Amount (g)
H-MFI-90 zeolite agglomerate powder	0-10[a]
γ-Al_2O_3	10-0[a]
Deionised water	37.5
Poly vinyl Alcohol	2.5
Acetic Acid	0.5

[a] *Various ratios of γ-Al_2O_3 and zeolite agglomerate powder were used*

The various washcoating suspensions were prepared in glass bottles with a screw lid which allowed the suspension container to remain airtight at all times, therefore preventing water evaporation. In order for the suspension temperature to be monitored, the suspension container was placed in a water bath and the temperature of the water bath was controlled. A magnetic stirrer (bar-bell) was placed inside the suspension container and used to stir the suspension. The apparatus is shown schematically in Figure 4.4.

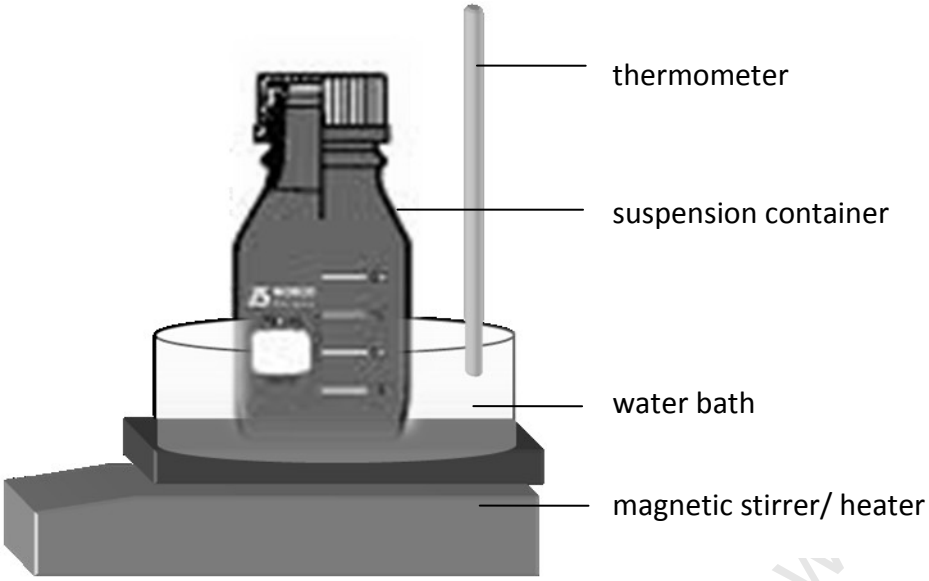

Figure 4.4: Experimental setup for washcoating suspension preparation.

4.3.2.1. Organic binder solution preparation

The inclusion of an organic binder was necessary to ensure that the suspension was homogenous. To prepare the binder solution, poly vinyl alcohol (PVA) and deionised water was added to the suspension container with the stirrer bar. The solution was stirred at a speed of 160 rpm and kept at 65 ˚C. Once the PVA had dissolved (after about 3 hours), the solution was left over-night without stirring at ambient temperature.

4.3.2.2. Zeolite/ γ-Al_2O_3 suspension preparation

In this step, the 'solids' (either zeolite powder or mixtures with γ-Al_2O_3) together with the acetic acid, were added to the organic binder solution. Again, the suspension container was held at 65 ˚C for 2 hours whilst stirring at 160 rpm, after which the suspension was stirred at ambient temperature for 3 days. A simple test was used to determine, qualitatively, whether the suspension was ready for coating. It comprised of checking the sharpness of the suspension 'edges' by swirling the suspension container and observing the edges of the suspension on the container walls. If the edges were smooth, the suspension was considered homogenous and ready for coating. In contrast, if the edges were jaggered, the suspension required further homogenization by continuous stirring at room temperature or, alternatively, the suspension was not of good quality.

4.3.3. Plate masking

Before coating the microchannel reactor plates, the inlet and outlet ports were covered using a polymer tape ('selo-tape') as shown in Figure 4.5 to prevent suspension coating these areas.

Figure 4.5: Masking of microchannel reactor plate ports.

The plates were placed on paper toweling and tape was applied to the inlet and outlet ports. The edge of the tape was placed as close to the microchannels as possible to ensure the amount coated was reproducible. The sides of the tape were then pressed down with a small spatula to ensure that no suspension could seep under the tape. The sides parallel to the length of the channels need not be taped since this would hinder the excess suspension being removed in the later, catalyst coating stage. Port covering was not required for the coating test plates since these plates did not have inlet or outlet ports.

4.3.4. Catalyst coating

In this step the catalyst was coated onto the stainless steel plates. To coat a plate, an amount of suspension was placed in the middle area of the channels as shown in Figure 4.6. It was important that there was sufficient suspension since adding more at a later stage would affect the quality of the washcoat. A scraper which consisted of a sharp metal blade was used to remove the excess suspension. Half of the suspension was scraped from the middle of the suspension pool to the one end of the microchannels (1), ensuring that the suspension had reached and completely filled the ends of all channels. This was repeated on the other side (2). Finally, the suspension was scraped once over the whole length of the plate (3), such that the channels were left full of coating suspension.

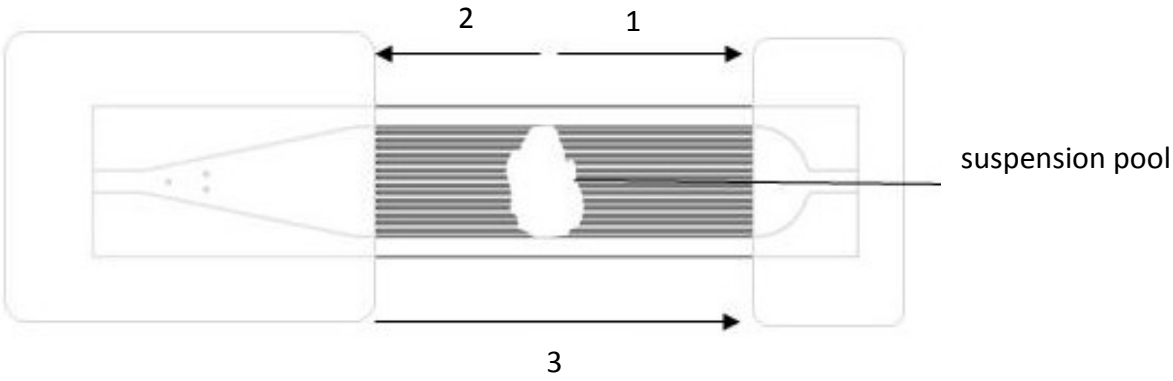

Figure 4.6: Method used to coat the microchannels with suspension.
[1-3 indicates the order and direction in which the suspension was scraped]

4.3.5. Drying and calcination

Once the plates had been coated with suspension, the plates were left to dry at ambient conditions. As the coating dried, it changed from a clear to a whiter colour. A homogeneously coated plate dried evenly from the outside edges to the centre.

After the coating was dry, the tape was removed, and the plates were calcined. When a large number of plates were calcined, the plates were stacked as shown in Figure 4.7. Magnesium oxide separators which were shaped as half pipes, about 5 cm long and 1 cm wide were used to separate these plates.

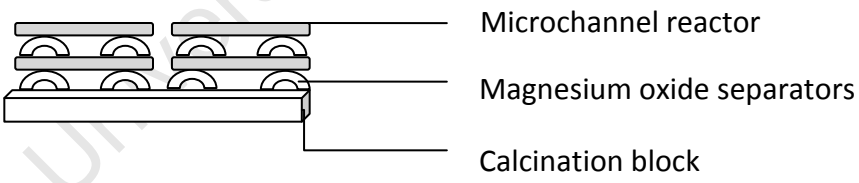

Figure 4.7: Calcination of coated plates setup.

The plates were calcined to remove the organic binder, acetic acid and water; and thus to leave only the remaining 'solids' coating on the microchannels. The calcination temperature is largely dependant on the type of catalyst used and should be adjusted accordingly. For the zeolite coatings, the same final temperature (600 °C) was used as for the γ-Al_2O_3 coatings. Figure 4.8 shows the calcination temperature programme used.

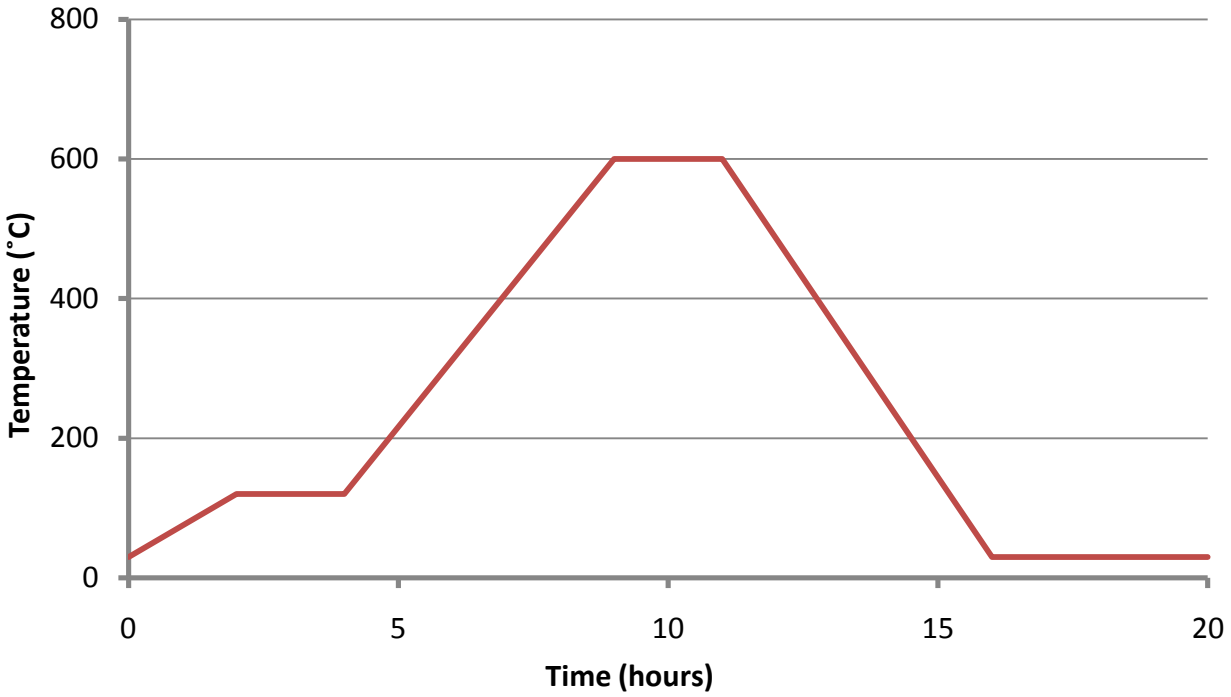

Figure 4.8: Temperature programme for calcination of coated microchannel reactor plates (holding temperatures at 120˚C and 600˚C for 2 hours).

4.3.6. Cleaning and weighing of coated plates

Any catalyst found on the plates in any area other than the channels had to be removed. The plates were cleaned using a soft instrument (e.g. ear care cotton buds) which would not remove any of the metal oxide layer since this would influence the plate weight. The plates were then weighed to the 4th decimal place and the catalyst loading determined, by comparison to the unloaded plate weights.

4.3.7. 'Ex-situ' preparation of simulated washcoat

In order to check whether or not the washcoating procedure reflected the original catalytic properties of the zeolite, a sufficient quantity of washcoat was prepared separately for loading into a conventional laboratory-scale fixed-bed reactor (Section 4.5.1). The excess suspension which was not used to coat the plates, was spread over a ceramic tile and left to dry overnight. Once dry, this coating was scraped off using a metal spatula and calcined according to the

calcination temperature programme used for the coated plates (Figure 4.8). Once calcined, the catalyst was ground using a pestle and mortar to form a granulate that could be charged to the fixed-bed reactor.

4.4. Washcoat suspension characterization

The suspension was characterized by measuring the particle size of the solids in the suspension, the suspension viscosity, and the pH.

4.4.1. Particle size

The particle sizes of both the original zeolite crystallite agglomerates and γ-Al_2O_3 powders, milled powders as well as the suspension particle size were determined using a Malvern Mastersizer. Approximately 2 g of the suspension or powder, 10 ml sodium-hexa-meta-phosphate (dispersant) and 5 drops of a Tritronex® solution (dispersant) were gently mixed together before adding dropwise to the Mastersizer's water bath. The obscuration was set between 20 - 30 % for consistency. Mild ultrasonification was applied throughout the analysis to prevent flocculation.

4.4.2. Suspension viscosity

The viscosity of the suspension was measured on the excess suspension after coating the plates, using a Brookfield DV-II viscometer with spindle number 63. The viscosity was recorded at shear rates of 50, 100, 150 and 200 s^{-1} with the power rating being between 50 and 90%. To measure the viscosity, 30 ml of the suspension was decanted into a smaller sample container (50 ml) and the viscosity was measured after initiating spindle rotation and the viscosity reading had stabilised. Care was taken to ensure that the amount of suspension added, size of the sample container, time of spindle revolutions to record the viscosity, and location of the spindle in the suspension was kept as constant as possible since these external factors influenced the final viscosity reading.

4.4.3. Suspension pH

The pH of the suspension was measured using a conventional pH meter calibrated with pH 4 and pH 7 buffer solutions.

4.5. Coating characterization

4.5.1. Preparation of coating powder

To perform X-ray diffraction and BET surface area analyses of the coating, a greater amount of coating was required than that which could be deposited onto a single test plate. The samples required for these analyses were therefore prepared using the modified method for 'ex-situ' layer materials as described in Section 4.3.7.

4.5.2. X-ray diffraction analysis

X-ray diffraction (XRD) analysis was undertaken using the ground coating prepared by the method described in Section 4.3.7. Ambient temperature powder X-ray diffraction measurements were carried out using a Bruker D8 spectrometer equipped with a Cu Kα radiation source in standard Bragg-Brentano geometry using a Ni filter at the detector. The scan range was 5 – 70 $^{o}2\theta$ in 0.02 steps.

4.5.3. BET surface area analysis

The BET surface area measurements by nitrogen adsorption were conducted using the ground coating prepared as described in Section 4.5.1. A Micromeritics Gemini 2375 instrument was employed on samples pretreated overnight at 120 ˚C under N_2 flow to remove water and other adsorbed volatile compounds from the catalyst.

4.5.4. SEM and EDX

The morphology of the coated plates, original zeolite powder, and cross-sectional view of microchannel plates were examined with a JEOL scanning electron microscope (SEM) operated at 6 kV, a working distance of 10 mm and various magnifications. In-situ EDX (Energy-dispersive

X-ray spectroscopy) of the coating was performed to obtain the elemental composition of the coating. Powder samples were gold-coated to prevent the powder from being mobile in the SEM vacuum chamber.

The washcoating thickness and distribution was evaluated by taking a cross-sectional image of the microchannel plate, for which it was required that the plate was embedded in a block resin. A smaller plate (cut shorter to 1 cm long) was coated and calcined as described in Section 4.3. The plate was mounted in a mould and embedded in a cast that consisted of a combination of polyset and Bakerset. Thereafter the cast block was ground and polished which resulted in the block exposing the plate shown from the side, as in Figure 4.9.

Figure 4.9: Plate embedded in a cast block of resin to evaluate the coated microchannel plate in cross-section.

4.5.5. Coating adhesion

In order to test the quality of the suspension and coating properties, the adherence of the washcoat to the stainless steel microchannel test plates was evaluated by a drop test (Zapf et al., 2006) and ultrasonification (Yasaki et al., 1993) (Section 2.4.4.3). Catalyst mass lost was recorded after each adhesion test and the percentage calculated using Equation 4.1.

$$\text{Weight loss (\%)} = \frac{(\text{Weight of coated plate} - \text{Weight after adhesion test}) \ \text{x} \ 100}{(\text{Weight of coated plate} - \text{Weight of uncoated plate})}$$

Equation 4.1: Determination of coating weight loss after adherence testing.

4.5.5.1. Drop test

The drop test has been developed as an adherence test to measure the mechanical stability of the coating (Zapf et al., 2006) as shown schematically in Figure 4.10. A microchannel plate was weighed and then attached to a stainless steel block (720 g) which fell 55 cm down a metal guide rod onto the stainless steel base. This was repeated 15 times and the weight of the plate recorded again thereafter. The amount of weight lost was the parameter used to asses the quality of adhesion.

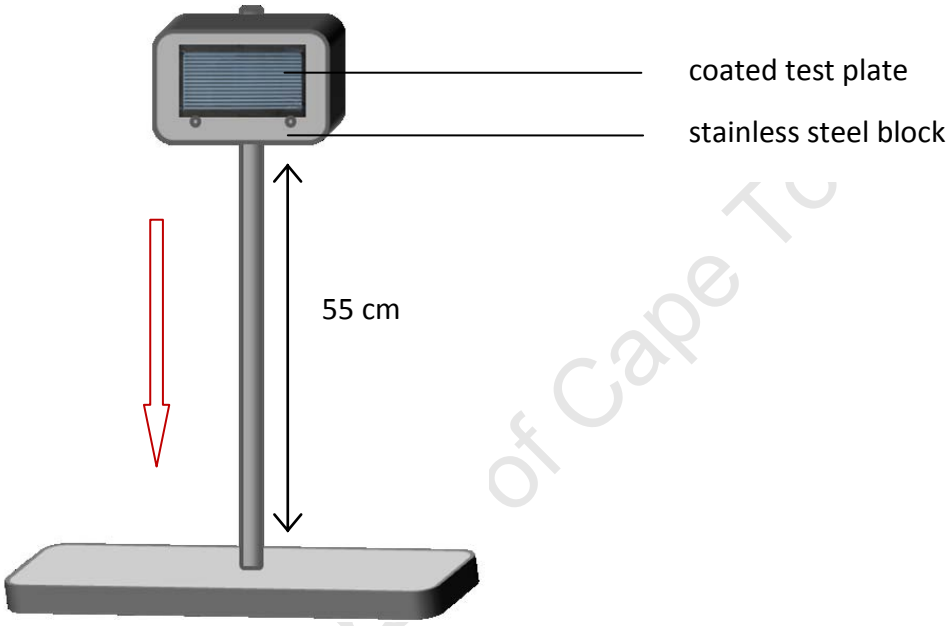

Figure 4.10: Drop test experimental apparatus.

4.5.5.2. Ultrasonification

An alternative adherence test was ultrasonification (Yasaki et al., 1993). In some instances, the plates were further tested for adhesion strength by this test. The coated plate was placed in a petroleum ether ultrasonic bath for 1 hour followed by placement in an isopropanol ultrasonic bath for another hour. Petroleum ether was chosen as a solvent to be consistent with the method developed by Yasaki et al. (1993) whilst the isopropanol solvent was chosen due to it being one of the reagents used in the test reaction.

4.5.6. Evaluation of microchannel plates after test reaction

In order for the microchannel plates to be evaluated after the test reaction, the microreactor was cut open along the laser welding seams on either side using a hack-saw.

4.6. Reaction experimental apparatus

A process flow diagram of the experimental apparatus used in the alkylation reaction to test the catalytic properties of the washcoating is illustrated in Figure 4.11. The apparatus is made from SS 316 stainless steel and individual parts (fittings, valves etc.) were from Swagelok^{TA}.

4.6.1. Nitrogen supply

Nitrogen was used to activate the zeolite catalyst in-situ and pressurise the reactor. The nitrogen was supplied from a pressure cylinder and passed through a filter (F-1) to remove any possible solids entrained in the line. The pressure regulator, PR-1, regulated the pressure when pressurizing the reactor and controlling back pressure during the experiments. Pressure regulator, PR-2, regulated the pressure of nitrogen being supplied to the mass flow controller, MFC-1 (Brooks). As a safety precaution to protect the mass flow controller; the check valves (CV-1 and CV-2), as well as the guard catch pot (GCP-1) were installed to prevent any liquid backflow from the reactor in the event of downstream line blockages.

4.6.2. Liquid feed (*m*-cresol and isopropanol)

A 1:1 molar ratio mixture of liquid *m*-cresol and isopropanol was provided in an enclosed feed vessel. A 2-decimal place balance connected to a laptop computer was used to constantly monitor the consumption of feed which was being pumped to the reactor in order to calculate the WHSV, as well as indicate any pump malfunction. An agitator was used to stir the feed mixture. This was necessary to prevent the isopropanol and *m*-cresol from separating into different liquid phases, as had been observed by Nagooroo (2011).

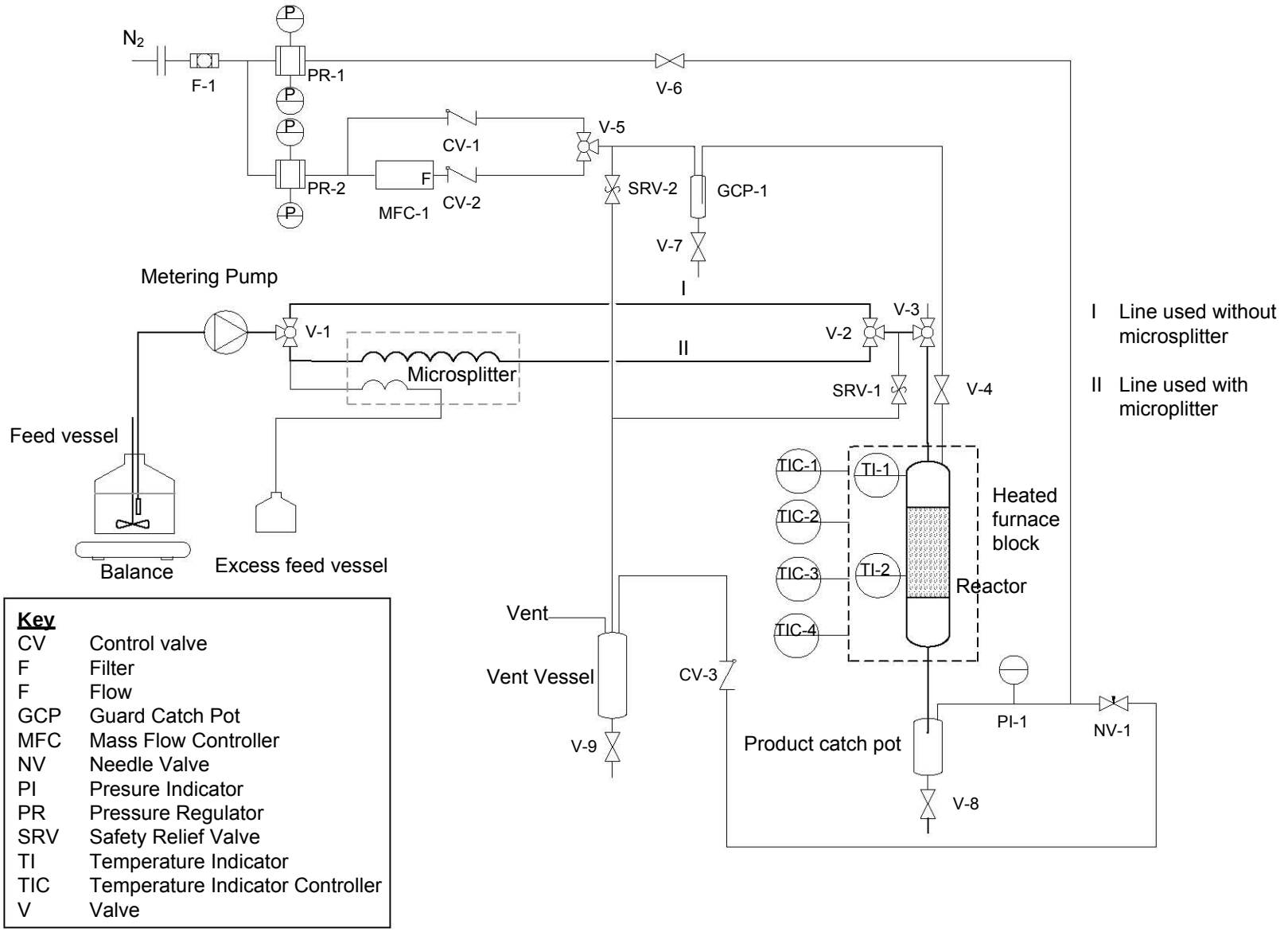

Figure 4.11: Process Flow Diagram of catalytic test apparatus

4.6.3. Metering pump

A duel piston Model 1500 HPLC pump (Scientific Systems Inc.) was used to pump the feed from the feed vessel to the reactor. This pump was capable of pumping a minimum flow rate of 0.001 ml/min. A filter was fitted to the line from the feed vessel to prevent any solid impurities from entering the liquid line which could damage the pump.

4.6.4. Microsplitter

To obtain flow rates below 0.001 ml/min, a microsplitter was connected in parallel to the by-pass line between valves V-1 and V-2 (Figure 4.11). The total feed pumped (0.001 ml/min) entered the microsplitter via the 'inlet port'. The metered flow passed right, through port 1 to be fed to the reactor (via V-2) (Figure 4.12). Port 2 was connected to the excess feed vessel. The excess feed was collected separately to enable better monitoring of the flow rate to the reactor. To adjust the split ratio, the dial on the microsplitter was turned clockwise to decrease flow to the reactor and increase flow to the excess feed pot. Use of the microsplitter enabled feed flow rates in the range of 0.0005 ml/min.

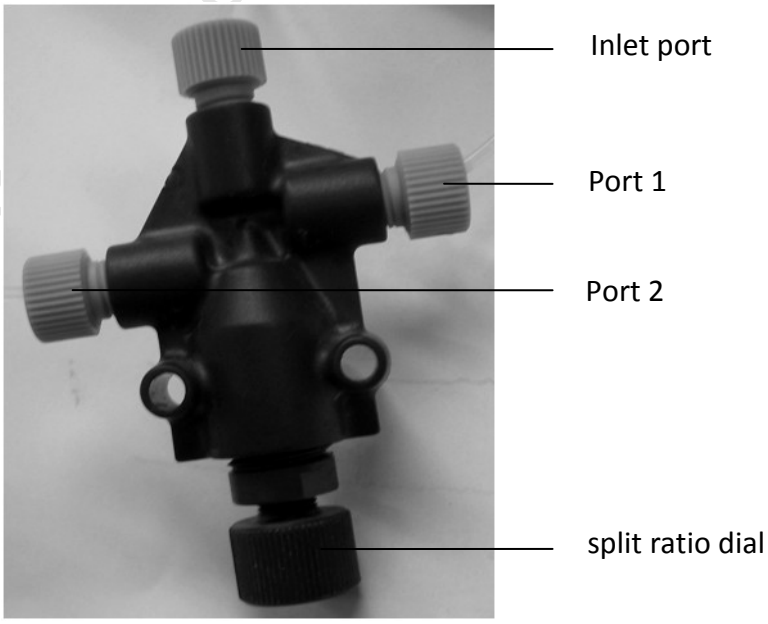

Figure 4.12: Microsplitter

4.6.5. Microchannel reactor

In order to form the microchannel reactor from the coated microchannel reactor plates, as well as incorporate the microchannel reactor into the experimental configuration shown in Figure 4.15 a unique assembly is required.

4.6.5.1. Microchannel reactor assembly

Once coated, the two microchannel reactor plates (Figure 4.13a) and the corresponding 1/8" tubing were assembled and welded together to form the microchannel reactor configuration with the circular microchannels (Figure 4.13b). The plates were laser welded together along the edges of the microchannel reactor and around the 1/8" tube connections. Pulsed-laser welding was chosen due to its accuracy and ability to confine the high temperature of the welding process to a very small area on the boundary walls of the microchannel reactor, thus avoiding degradation of the catalyst coating.

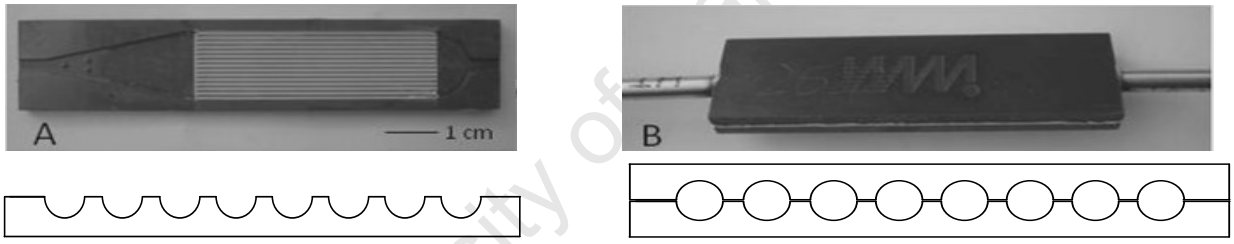

Figure 4.13: (a) Single coated microchannel reactor plate with half-pipe microchannels (b) Two microchannel reactor plates welded together to form microchannel reactor with tubular microchannels.

4.6.5.2. Microchannel reactor installation

The microchannel reactor, as configured in Figure 4.13b, was fitted into a heating block made up from brass sleeves as illustrated in Figure 4.14 so as to provide good heat conductivity and ensure an isothermal temperature profile in the microchannel reactor. Sleeve S-1 has a circular key-hole cut to accommodate the 1/8" stainless steel tubes at the microchannel reactor inlet/outlet, whereas sleeve S-2 has a rectangular key-hole cut in order to incorporate the microchannel reactor body. Two 4 cm long S-2 sleeves were used to enclose the microchannel reactor body and one 8 cm long S-1 sleeve was placed on either end of the microchannel reactor to enclose the 1/8" tubing. To keep the sleeves in place, two 25 cm long metal rods

were threaded through holes A and B, and tightened on either end with screws. (Figure 4.15 shows the overall assembly). The smaller hole near the centre of the sleeves acts as a thermowell which allowed a thermocouple to be moved up and down to measure the temperature and determine the temperature profile of the microchannel reactor.

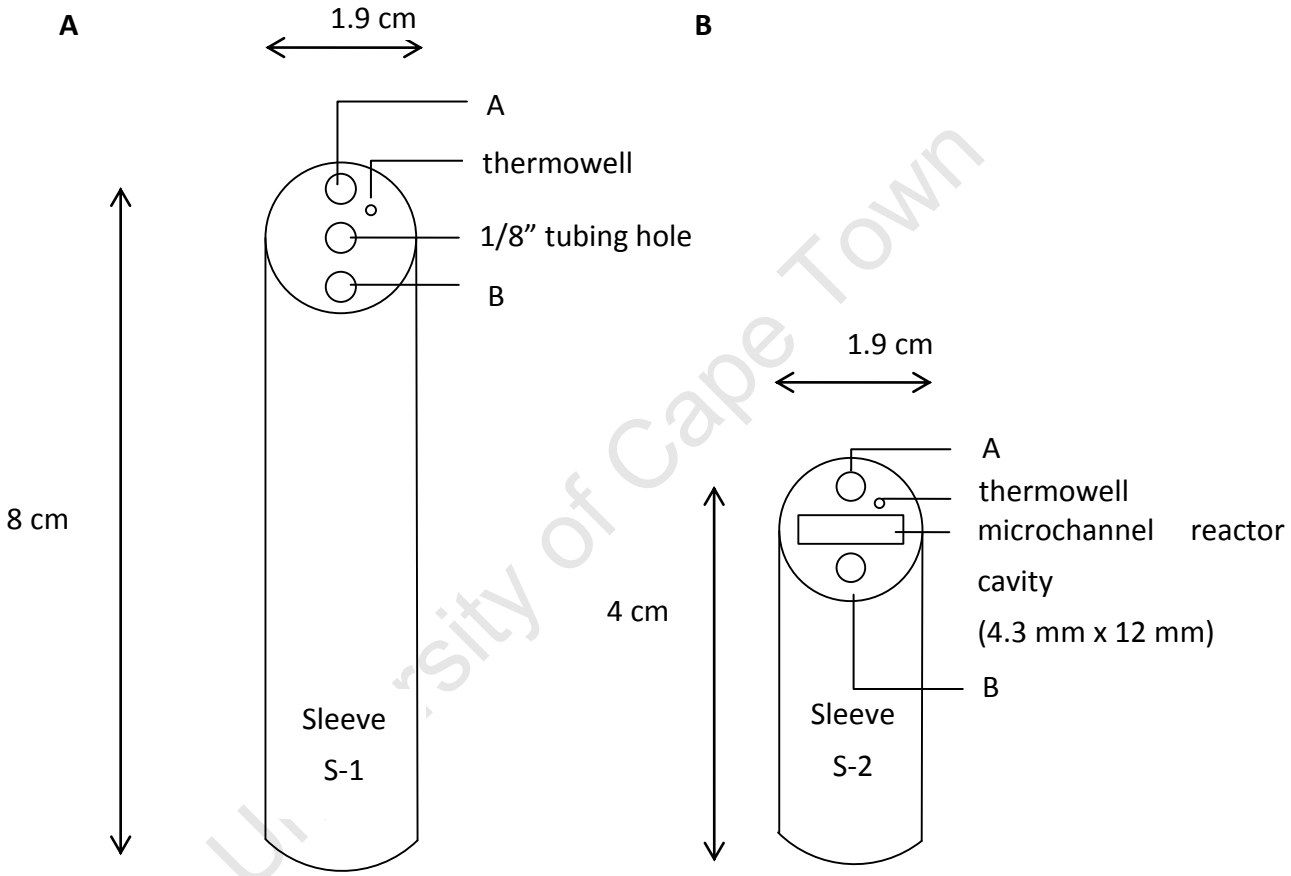

Figure 4.14: Metal sleeves used to fit the microchannel reactor. (a) to accommodate the 1/8" tube extensions (b) to accommodate the microchannel reactor body.

4.6.5.3. Vapouriser

A vapouriser shown in Figure 4.15 was used to vapourise the liquid feed stream and preheat the vapour to reaction temperature. The 17 cm long stainless steel tube of internal diameter of 15.75 mm was filled with silicon carbide (grit size = 20 and ∅ = 1.3 µm) to increase heat transfer. Glass wool was placed at the bottom of the vaporizer to prevent any silicon carbide falling into the microchannel reactor. The temperature of the vapouriser was adjusted so that a

smooth temperature profile ranged from slightly above ambient temperature at the inlet, to reaction temperature at the outlet, to ensure steady evaporation.

4.6.5.4. Assembly of microchannel reactor, vapouriser and outlet port

Once the microchannel reactor body had been placed in the sleeves and the metal rods were in place, the vapouriser and outlet tube were connected to form the complete reactor configuration shown in Figure 4.15. This was achieved by two 1/8" Swagelok^{TA} fittings on either end of the 1/8" microchannel reactor extension tubes to join to the vapouriser and outlet tube.

4.6.5.5. Reactor head

The reactor heads were identical in both the microchannel reactor and fixed-bed configurations (Figure 4.15 and Figure 4.16). The heads were mounted onto the reactor tube by Swagelok^{TA} VCR fittings. The heads contained the N_2 inlet (for drying and activation), liquid reagent inlet and top thermocouple.

The top thermocouple's tip was situated at the top of the vapouriser and measured the temperature of the feed entering the vapouriser. This was necessary to ensure that the temperature of the incoming feed was below the boiling point for the feed at the specific reaction pressure.

4.6.6. Fixed-bed reactor

4.6.6.1. Fixed-bed reactor body

The tubular fixed-bed plug flow reactor, illustrated in Figure 4.16, consisted of a 700 mm, ¾" stainless steel tube with an internal diameter of 15.75 mm. The same reactor head as for the microchannel reactor configuration, discussed in Section 4.6.5.5, was used.

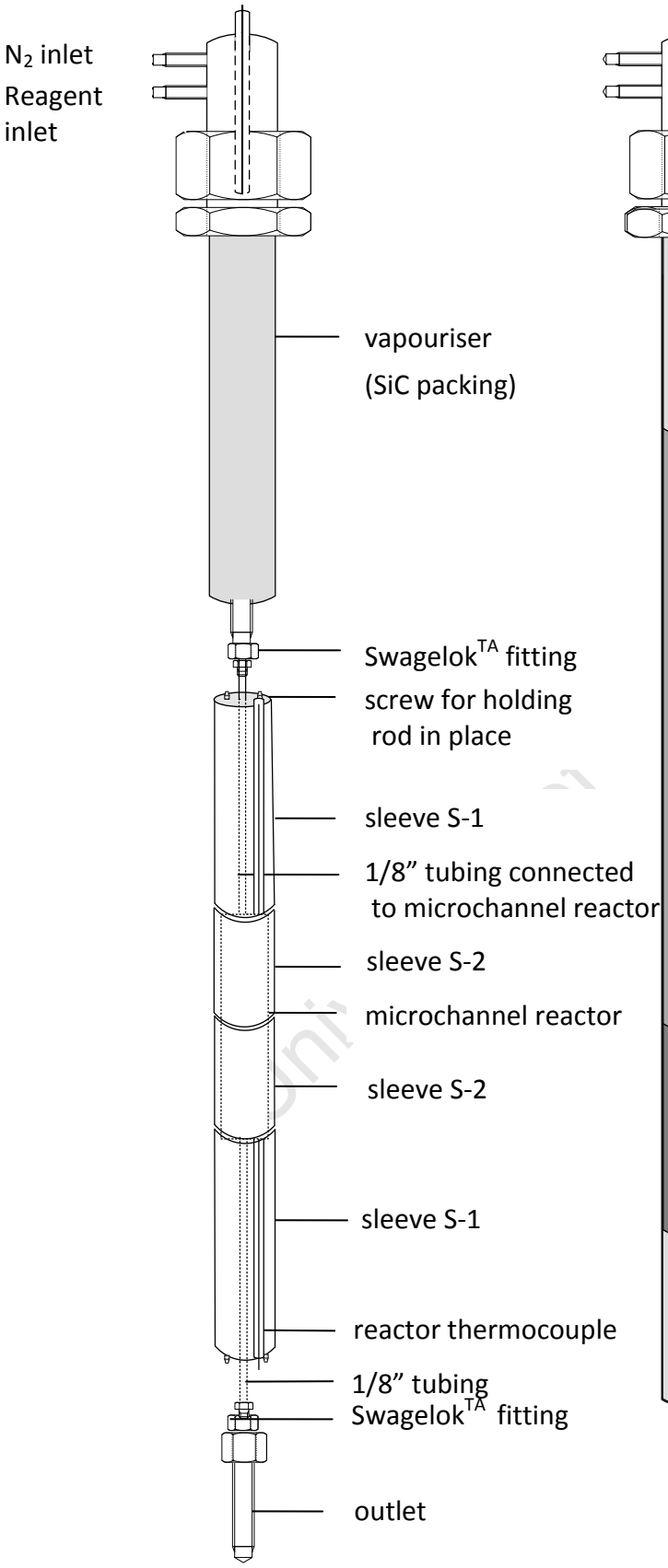

Figure 4.15: Microchannel reactor experimental configuration.

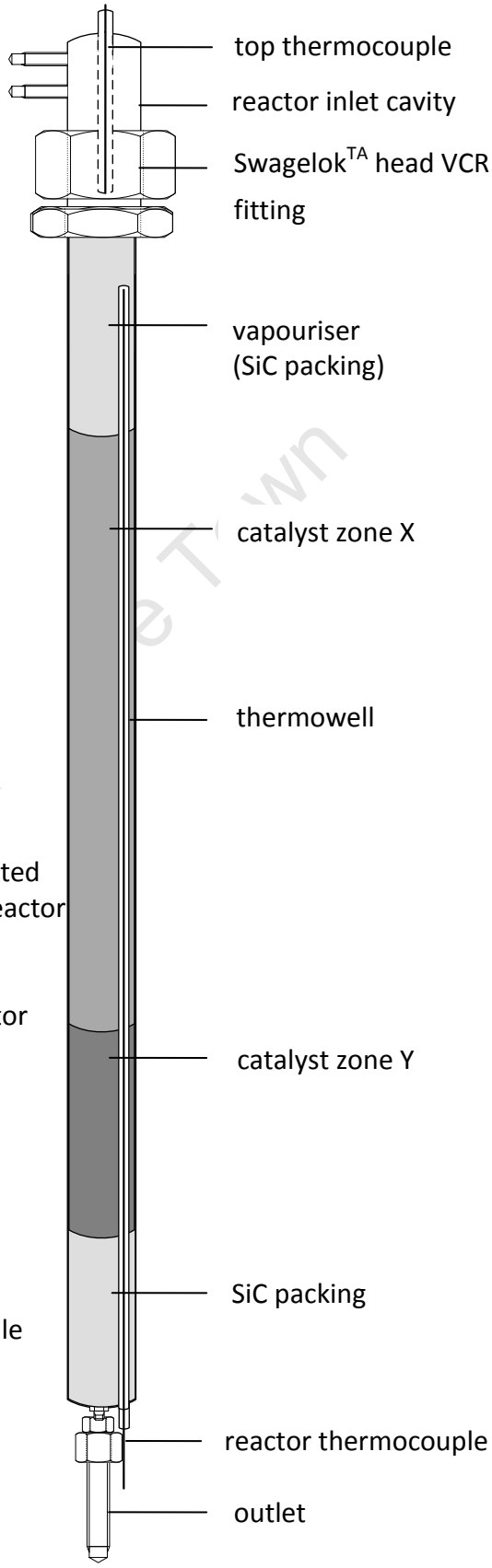

Figure 4.16: Fixed-bed reactor experimental setup.

4.6.6.2. Catalyst packing

In the fixed-bed reactor, the zeolite catalyst and silicon carbide were packed into various zones as shown in Figure 4.16 . Inert silicon carbide (grit size 20 and particle size ∅ = 1.3 µm) was used as a catalyst diluent and for the other packings. The top silicon carbide packing zone of approximately 5 cm formed the preheating vapourisation zone of the reactor. In this zone the liquid feed was vapourised and heated to reaction temperature as discussed for the microchannel reactor configuration (Section 4.6.5.3).

The catalyst bed was divided into two zones which had different catalyst:SiC ratios. In the first catalyst zone, X, the volume ratio was 1:8 and in the second catalyst zone, Y, the volume ratio was 1:1. Dilution of the catalyst bed with SiC was done to:

- Improve the radial heat exchange by extending the length of the catalyst bed and improve the radial mixing in the reactor given the endothermic and exothermic nature of the main reactions (dehydration of the isopropanol and alkylation of the *m*-cresol, respectively).
- Decrease the effective particle size within the catalyst bed when using catalyst extrudates and thus improve the hydrodynamic flow properties.
- Limit any opportunity for reagents and product channeling.

Catalyst zone X at the top of the reactor was diluted to a greater extent to limit the cooling down by the endothermic isopropanol dehydrogenation reaction at the top of the catalyst bed.

4.6.7. Reactor heating zones and temperature profile

The reactors shown in Figure 4.15 and Figure 4.16 were inserted simply into cylindrical cores of a furnace comprising a brass block of 80 mm x 80 mm cross-section and of 360 mm length. Four heating bands were arranged along the length of the brass block to make up four heating zones which were individually monitored and controlled to ensure that the temperature in the catalyst bed was close to isothermal. To measure the reactor temperature profile, a thermocouple was moved up and down within an axial thermowell (1/8" stainless steel tubing) extending from the bottom to the top of the reactor body or, in the case of the microchannel configuration within the brass sleeves making up the reactor 'body' (Figure 4.15 and Figure

4.16). Typical temperature profiles obtained in the microchannel and fixed-bed reactor configuration at a target temperature of 275 ˚C are shown in Figure 4.17.

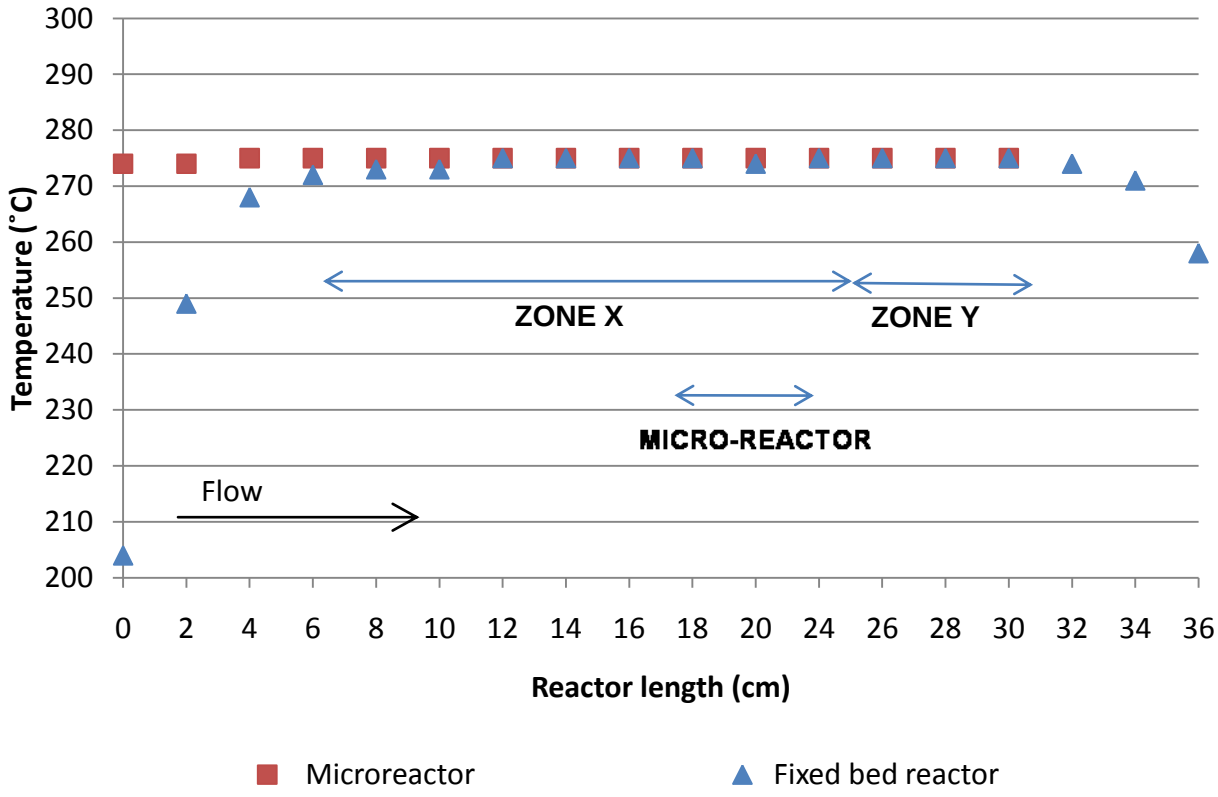

Figure 4.17: Temperature profiles in microchannel and fixed-bed reactors. (Reactor length at 0 cm depicts the top of the reactor preheat tube.)

4.6.8. Sample catch pot

The gaseous product stream leaving the reactor passed through a cooling coil (air cooled) to condense the product stream for collection in a 100 ml sample catch pot. Product sampling was done at regular time intervals depending on the WHSV. To sample, valve V-7 was opened and the sample catch pot drained of all its contents taking care not to depressurize the system in the process.

4.7. Reactor operation

Once the microchannel reactor had been assembled (Figure 4.15), or alternatively, the fixed-bed reactor catalyst loaded (Figure 4.16), the reactor could be incorporated into the

experimental rig and the experimental operation initiated. This section provides the details of the start-up, on-line, and shut-down procedures.

4.7.1. Reactor inclusion

To connect either the microchannel reactor (Figure 4.15) or fixed-bed reactor (Figure 4.16) configuration to the rest of the experimental rig (Figure 4.11), the following connections were required:

- Nitrogen reactor inlet connected to nitrogen line (1/8" VCR)
- Reagent reactor inlet connected to incoming feed line (1/8" VCR)
- Product reactor outlet connected to outlet line (1/8" VCR)
- Top thermocouple connected to temperature indicator unit (1/8" Swagelok^{TA})
- Reactor thermocouple inserted into thermowell

4.7.2. Leak test

To test the experimental setup (Figure 4.11) for leaks, the reactor was pressurized with nitrogen according to the following procedures below:

4.7.2.1. Fixed-bed reactor

Valves V-3, V-6 and V-8, and needle valve NV-1 were closed to isolate the reactor. Pressure regulator, PR-2, was opened and the reactor was pressurized to 10 bar. The pressure was monitored using pressure indicator, PI-1 for 2 hours and soapy water was applied to all the joints to determine whether there was any leak in the reactor lines. If the pressure in the reactor did not drop, and there was no gas leak from the joints, the reactor was deemed "pressure tight".

4.7.2.2. Microchannel reactor

The microchannel reactor configuration shown in Figure 4.15 had an additional Swagelok^{TA} fitting before and after the microchannel reactor plates. To test whether these fittings were pressure tight, a pressure test was performed with the microchannel reactor outside the heating block. A valve was fitted to the bottom outlet of the reactor, after the second Swagelok^{TA} fitting. The inlet connections to the reactor head were connected as described in

Section 4.7.1. The microchannel reactor was pressurized from the top to a pressure of 5 bar. The fittings were checked with soapy water, and the pressure was monitored to determine whether there was any loss of pressure over a 2 hour time period. If no pressure loss occurred, the reactor was deemed “pressure tight”.

The valve fitted to the reactor outlet was then removed and the reactor was inserted into the heating block. The reactor outlet connection was fitted and the reactor was reconnected as described in Section 4.7.1. To check whether there was a leak in the reactor system, the same procedure was implemented as in the fixed-bed reactor leak test (Section 4.7.2.1), to increase the pressure in the reactor to 5 bar. If there was no decrease in reactor pressure, and no gas leak observed from applying soapy water, then the reactor was deemed “pressure tight”.

4.7.3. Catalyst drying and activation

The catalyst was dried and activated by flowing nitrogen through the reactor. For the fixed-bed reactor a nitrogen flow rate of 50 ml/min was used, whereas with the microchannel reactor, a nitrogen flow rate of 10 ml/min was used.

A mass flow controller, MFC-1, was used to control the nitrogen flow rate. Valve V-4 was opened, and the 3-way valve, V-5, set to induce flow through the mass flow controller, with the pressure regulator, PR-2, set to 10 bar and the mass flow controller set to the corresponding flow rate depending on the reactor configuration in use. With valve V-8 open, catalyst drying and activation was conducted at atmospheric pressure.

The temperature programme applied for the catalyst drying and activation is presented in Figure 4.18. In the drying phase (0 - 4.5 hours), the moisture was slowly removed from the catalyst. In the activation phase, other impurities adsorbed onto the catalyst were removed. This was done by increasing the reactor temperature to 350 ˚C and holding this temperature for 4 hours. After the catalyst activation, the reactor temperature was lowered to the initial operating temperature (275 ˚C).

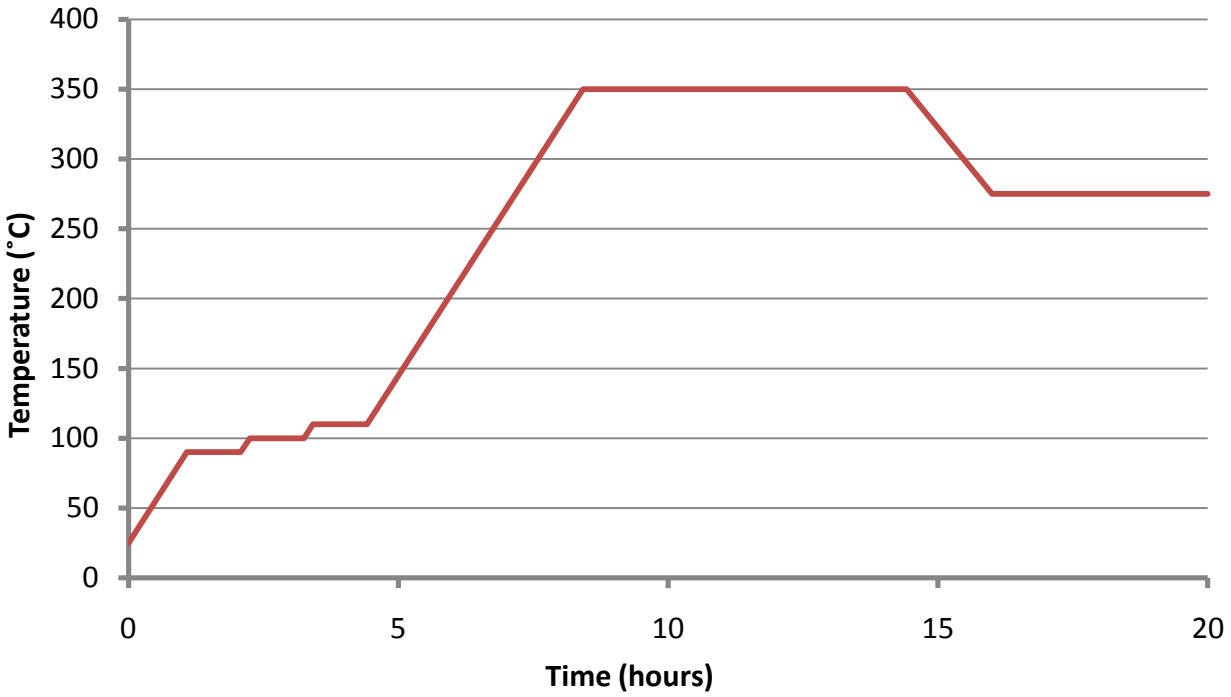

Figure 4.18: Temperature programme for catalyst drying, activation, and reaction start up (275 ˚C).

4.7.4. Start up procedure

Once the drying and activation phase was complete, the nitrogen flow was stopped by, switching off the mass flow controller (MFC-1), closing the pressure regulator (PR-2) and closing valve V-5. To release any build up in pressure, valve V-7 was briefly opened. Finally, valve V-4 was closed (the importance of V-4's function is discussed in Appendix C).

4.7.4.1. Pressurisation of reactor

Pressurisation of the reactor was undertaken by slowly pressurising with nitrogen from the bottom of the reactor. Pressure regulator, PR-1, was opened and set to the reaction pressure with needle valve NV-1 set sufficiently open to allow a small continuous nitrogen flow whilst still maintaining at desired pressure at PI-1. The reaction pressure was adjusted according to the indication of the pressure indicator, PI-1 on the outlet line from the product catch vessel.

4.7.4.2. Priming pump and feed line

To maintain trouble-free pump operation, a 20% isopropanol/distilled-water solution was continuously circulated through the rear of the pump heads. This flushing solution serves only to 'wash' the pump piston, and its flow path is independent of the principal pumping path. To prime this solvent line, a syringe was connected to the outlet tubing and solvent was drawn from the solvent reservoir until the inlet line was primed, after which the syringe was removed and the outlet tubing connected to the solvent reservoir so as to ensure a closed recirculation loop for the head flushing solvent.

The pumping circuit itself was primed sequentially from the suction line to the reactor feed line. This was done by attaching a syringe to the pump purge outlet and drawing approximately 15ml of feed solution under syringe suction, followed by initiation of the pump prime function until all air bubbles were cleared from both the feed and purge lines, after which the pump prime function was halted, the purge valve closed and the syringe removed. To prime the feed line to the reactor, valves V-1 and V-2 were set to bypass the microsplitter, valve V- 3 was opened and the pump prime mode initiated. After clearing any bubbles present in the fluid exiting the purge stream outlet at the base of valve V-3, the valve was switched so that the feed was directed toward the reactor. Once the temperature of the top reactor thermocouple indicating the presence of feed at this point, dropped, the pump prime function was halted and the required flow rate set.

4.7.5. Product sampling procedure

Product samples were collected batch-wise at regular time intervals depending on the WHSV applied. The frequency of sampling for the respective flow rates is stated in Section 4.11. To collect a sample, valve V-8 (Figure 4.11) was opened slowly and the product drained until the product vessel was empty. The samples were collected in glass sample vials with poly-tops.

At each set of reaction conditions, approximately 5 to 6 samples were taken after steady state had been established to ensure sufficient accuracy of the averaged data. The samples were analysed of offline gas chromatography, the details of which are presented in Section 4.8.

4.7.6. Shut-down procedure

To shut-down the experimental test, the following procedure was followed (Figure 4.11):

- The feed pump was switched off and valve V-3 was closed.
- The reactor pressure was released to atmospheric pressure by closing pressure regulator, PR-1, and opening the needle valve, NV-1, to vent the controlling nitrogen pressure.
- The reactor temperature controllers were switched off and the reactor flushed overnight with nitrogen via valve, V-4.

4.8. Product analysis

The product samples were analysed by gas chromatography using a special "positional isomers" column (Table 4.7) to correctly quantify the various thymol isomers. A Varian 4800 GC was employed together with a Varian CP-4800 autosampler and flame ionization detector (FID). The specific settings of this GC are given in Table 4.7.

Table 4.7: Product chromatographic analysis.

Column	Supelco 24310
Type	Wall coated fused silica capillary column
Stationary phase	A-DEX 120[a]
Length	30 m
Internal diameter	0.25 mm
Film thickness	0.25 µm
Injector temperature	300˚C
Detector temperature	320˚C
Column temperature programme	50˚C, 30˚C/min to 170˚C (holding time 2 min), 0.5˚C/min to 174˚C, 40˚C/min to 220˚C (3 min holding time)
Carrier gas	171 ml/min H_2
Column flow (ml/min)	0.5
Split ratio	340
Sample volume injected	5 µl
Insertion method	Automatic

[a] *20% permethylated α-cyclodextrin (a crown ether) in 35% diphenyl/ 65% dimethyl siloxane*

To analyse the product samples, 0.4 ml of product sample and 0.8 ml acetone was pipetted into an autosampler vial (1.5 ml). The acetone was used as a diluent to ensure better comparability between the various samples analysed. The peak identification which was done by Nagooroo, (2011) was used as a basis with a detailed description of the peak identification methods used described in Appendix D.

4.9. Chromatographic data workup

4.9.1. Correction of peak areas and response factors

The chromatogram peaks are a function of the amount of carbon associated with a peak and the intensity of the carbon atom ionisation of a particular species. The GC Flame Ionisation Detector (FID) signal integrator calculates the peak areas. The intensity of the FID signal produced for a certain carbon atom is strongly dependent on the type of atoms it is bonded to. Carbon bonded to oxygen gives a lower FID signal of only 55% in comparison to the carbon bonded to carbon and carbon bonded to hydrogen which gives equal FID signals. To compensate for the lower intensity of the carbon atoms bonded to oxygen, an average response factor (f_i) is used to obtain a "corrected peak area" which gives the actual amount of carbon associated with a particular peak, i.e. the carbon atom or carbon mass is proportional.

4.9.2. Calculation of response factors

A response factor is calculated for each compound by determining the ratio of total carbon atoms relative to the response of these carbon atoms. For the response of a carbon atom with a single bond of an oxygen atom, the value determined by the Centre for Catalysis Research, UCT, is 55. The response factor for thymol is calculated in Equation 4.2 as an example.

$$f_{thymol} = \frac{\text{number of carbon atoms in thymol}}{\text{response of carbon atoms in thymol}} = \frac{10}{9 \times 1 + 1 \times 0.55} = \frac{10}{9.55}$$

Equation 4.2: Calculation of response factor for thymol (f_{thymol}).

4.9.3. Corrected peak areas (PAC)

The original peak area which was obtained from the chromatogram was multiplied by the response factor to calculate the corrected peak area of oxygen compounds, i (PAC_i). Keeping the example of thymol, the corrected peak area (PAC_{thymol}) is calculated from the peak area (PA_{thymol}) as shown in Equation 4.3.

$$PAC_{thymol} = PA_{thymol} \times f_{thymol} = PA_{thymol} \times \frac{10}{9.55}$$

Equation 4.3: Calculation of corrected peak area thymol (PAC_{thymol}).

4.9.4. Molar corrected peak areas (PAM)

The corrected peak areas (PAC_i) were then converted to mol proportional values (PAM_i). A PAM_i was determined by the ratio of the corrected peak area relative to the number of carbon atoms in the specific molecule. An example of this calculation is shown in Equation 4.4.

$$PAM_{thymol} = \frac{PAC_{thymol}}{\text{Number of carbon atoms in thymol}} = \frac{PA_{thymol}}{9 \times 1 + 1 \times 0.55} = \frac{PA_{thymol}}{9.55}$$

Equation 4.4: Conversion of corrected peak area of thymol (PA_{thymol}) to mol proportional basis (PAM_{thymol}).

4.10. Conversion, product yield and selectivity calculations

The conversions, selectivities and yields at the various operating conditions needed to be calculated in order to evaluate the performance of the different catalyst preparations and different reactor configurations. All the calculations assume that all the *m*-cresol that entered the reactor also exited the reactor in the form of phenolic compounds that were detected by the FID. This allows for a phenol ring balance to be calculated.

4.10.1. *m*-Cresol conversion

The conversion of *m*-cresol was calculated using the mole proportional peak area of the unconverted *m*-cresol ($PAM_{m\text{-Cresol}}$) and the sum of the molar peak areas of the phenolic products (ΣPAM_i). Equation 4.5 illustrates this calculation.

$$X_{m-Cresol} = 1 - \frac{PAM_{m-Cresol}}{\sum_i^n PAM_i}$$

Equation 4.5: Calculation of the conversion of *m*-cresol.

4.10.2. Thymol Yield

The molar yield of a particular product was calculated by dividing the molar proportional peak area (PAM_i) by the sum of the molar peak areas (ΣPAM_i) of all the phenolic products present in the system i.e. the phenolic reactant and the phenolic products. Equation 4.6 illustrates this calculation.

$$Y_{thymol} = \frac{PAM_{thymol}}{\sum_i^n PAM_i}$$

Equation 4.6: Calculation of thymol molar yield

4.10.3. Selectivity

The molar selectivity of the various products was calculated by dividing its mol proportional peak area (PAM_i) by the sum of the mol proportional peak areas of all phenolic products which can be simplified to the ratio of the product yield relative to the *m*-cresol conversion. Equation 4.7 illustrates this calculation with thymol selectivity as an example.

$$S_{thymol} = \frac{PAM_{thymol}}{(\sum_i^n PAM_i) - PAM_{m-Cresol}} = \frac{Y_{thymol}}{X_{m-Cresol}}$$

Equation 4.7: Calculation of molar selectivity of thymol.

4.11. Catalytic testing programme

All catalyst tests in the fixed-bed reactor were carried out at a temperature of 275 ˚C and a pressure of 3 bar (abs), while the WHSV was varied (Section 4.11.1). In the case of the microchannel reactor test series, in addition to varying WHSV, the temperature was also varied between 275 ˚C and 325 ˚C (Section 4.11.2). Each experiment was initiated at a standard WHSV to monitor initial catalyst deactivation until a quasi-steady state was reached. Thereafter, space velocity was varied by altering the feed pump rate and allowing the system to stabilise for between 12 and 24 hours depending on the feed flow rate. After completion of a particular set of test conditions, the initial conditions were re-established to allow for an assessment of catalyst stability over the intervening period.

4.11.1. Fixed-bed reactor

In Table 4.8 - Table 4.10, fixed-bed catalytic test conditions are compiled for the H-MFI-90 powder, H-MFI-90 extrudates and the simulated washcoat, respectively. Bold table entries indicate initial standard conditions in all tables (Table 4.8 – Table 4.11).

Table 4.8: Fixed-bed operating conditions: H-MFI-90 granulate (5.83g).

Temperature (˚C)	**Pressure (bar, abs)**	**Flow rate (ml/min)**	**WHSV ($g_{m\text{-}cresol}/g_{Zeolite}h$)**	**Period of sampling (hrs)**
275	**3**	**0.16**	**0.96**	**1**
275	3	0.12	0.72	1
275	3	0.302	1.81	0.5
275	3	0.604	3.62	0.5
275	3	0.05	0.3	2
275	**3**	**0.16**	**0.96**	**1**

Table 4.9: Fixed-bed operating conditions: H-MFI-90 extrudates (5.83g).

Temperature (˚C)	Pressure (bar, abs)	Flow rate (ml/min)	WHSV ($g_{m\text{-}cresol}/g_{Zeolite}h$)	Period of sampling (hrs)
275	**3**	**0.16**	**1.2**	**1**
275	3	0.08	0.6	2
275	3	0.04	0.3	2
275	3	0.08	0.6	2
275	**3**	**0.16**	**1.2**	**1**
275	3	0.32	2.4	0.5
275	3	0.64	4.8	0.5
275	**3**	**0.16**	**1.2**	**1**

Table 4.10: Fixed-bed operating conditions: Simulated washcoating of 75% H-MFI-90 and 25% γ-Al_2O_3 (5.83g).

Temperature (˚C)	Pressure (bar, abs)	Flowrate (ml/min)	WHSV ($g_{m\text{-}cresol}/g_{Zeolite}h$)	Period of sampling (hrs)
275	**3**	**0.16**	**1.28**	**1**
275	3	0.15	1.2	1
275	3	0.037	0.3	2
275	3	0.227	1.81	0.5
275	3	0.454	3.63	0.5
275	**3**	**0.16**	**1.28**	**1**

4.11.2. Microchannel reactor

In Table 4.11 the catalytic test conditions are compiled for the microchannel reactor configuration containing a 75% Zeolite washcoat.

Table 4.11: Microchannel reactor operating conditions: Washcoating of 75 wt% Zeolite and 25 wt% γ-Al_2O_3 (0.0251 g).

Temperature (˚C)	Pressure (bar, abs)	Feed flowrate (ml/min)	WHSV ($g_{m\text{-}cresol}/g_{zeolite}h$)	Period of sampling (hrs)
275	3	0.001	1.85	24*
275	**3**	**0.002**	**3.71**	**12**
300	3	0.002	3.71	12
325	3	0.002	3.71	12
275	**3**	**0.002**	**3.71**	**12**

* for 43 hours on stream

5. Zeolite Washcoating

In order to incorporate the zeolite catalyst into the microchannel reactor configuration, a zeolite washcoating technique, specific to microchannel reactors, was developed to coat zeolites onto microchannel walls. The properties of a "directly-substituted" zeolite washcoating are presented, whereby the as-received H-MFI-90 powder is substituted for γ-Al_2O_3 powder used in the washcoating method of Section 5.1 (Zapf et al., 2006). The effect of suspension properties on the washcoat (Section 5.2), optimised suspension (Section 5.3), and other coating properties, such as the washcoat after test reaction, reproducibility, channel dimensions and variations to the Zapf et al. (2006) washcoating technique are also presented. A summary of the various suspensions considered is tabulated in Table 5.1.

Table 5.1: Experimental programme in respect of washcoating suspension composition.

Section	Name of suspension	Suspension Composition *				Zeolite particle size (μm)	Description
		Zeolite (g)	γ-Al_2O_3 (g)	Silica (g)	PVA (g)		
5.1	**Directly-substituted zeolite**	10	-	-	2.5	34	Original zeolite powder
5.2.1.3	**Zeolite - A**	10	-	-	2.5	11	Reduced particle size
5.2.1.3	**Zeolite - B**	10	-	-	2.5	7	
5.2.2.1	**Silica A**	10	-	2.5	2.5	34	Addition of silica binder
5.2.2.1	**Silica B**	10	-	2.5	0	34	
5.2.2.1	**Silica C**	10	-	1.25	1.25	34	
5.2.2.2	**Zeolite 100%**	10	-	-	2.5	34	Addition of γ-Al_2O_3 binder
5.2.2.2	**Zeolite 90%**	9	1	-	2.5	34	
5.2.2.2	**Zeolite 85%**	8.5	1.5	-	2.5	34	
5.2.2.2	**Zeolite 75%**	7.5	2.5	-	2.5	34	
5.2.2.2	**Zeolite 50%**	5	5	-	2.5	34	
5.2.2.2	**Alumina**	-	10	-	2.5	-	
5.3	**Zeolite 75% - A**	7.5	2.5	-	2.5	16	Optimised suspension
5.3	**Zeolite 75% - B**	7.5	2.5	-	2.5	8	

** No variation to the amount of distilled water (37.5 g) and acetic acid (0.5 g) added.*

5.1. Directly-substituted zeolite washcoating

The γ-Al_2O_3 washcoating method developed by Zapf et al. (2006) was used as the baseline or reference point for the development of the zeolite washcoating method. The zeolite crystal agglomerate powder (Figure 5.1a) was directly substituted for the γ-Al_2O_3 powder whilst keeping all other suspension additives identical to the method of Zapf et al. (2006), resulting in the zeolite washcoating depicted in Figure 5.1b. A summary of the washcoat suspension and coating properties is presented in Table 5.2.

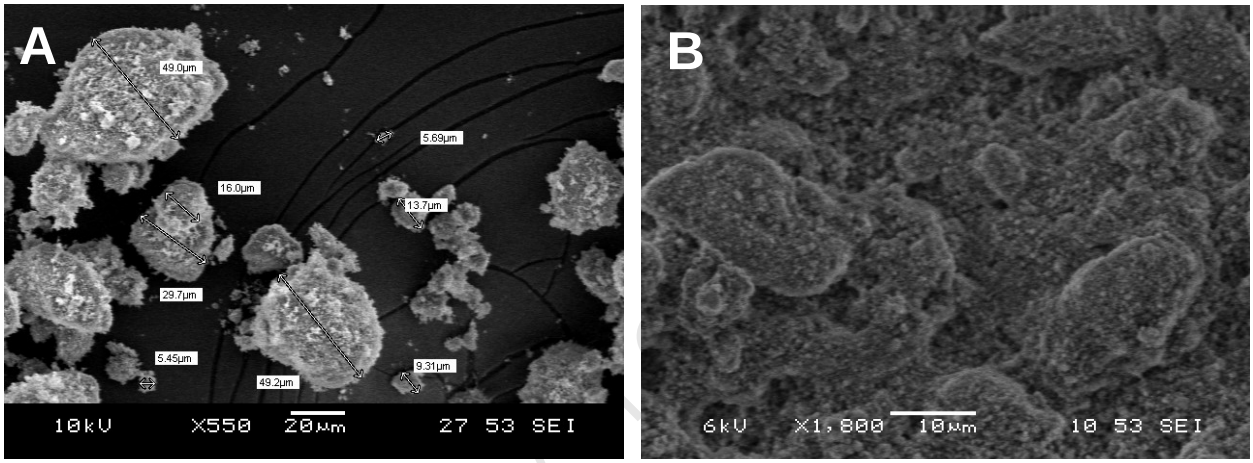

Figure 5.1: SEM image of (a) original H-MFI-90 zeolite catalyst agglomerate powder (b) directly-substituted zeolite washcoat.

Table 5.2: Suspension and coating properties of original zeolite powder and directly-substituted zeolite washcoating.

	Original zeolite powder [a]	Directly-substituted zeolite washcoating
Average particle size (µm)	34	14[b]
BET Surface Area (m^2g^{-1})	369	365
Viscosity (cP at 50 s^{-1})	-	1677
pH	-	3.1
Adherence test (% catalyst lost) [c]	-	8.1
Amount coated (g)	-	0.0430

[a] *Original zeolite crystal agglomerate powder*
[b] *Size of particles in suspension before coating*
[c] *Percentage mass loss of catalyst after drop tests.*

5.1.1. Particle size

Figure 5.1a depicts a SEM image of the original zeolite powder showing zeolite crystal agglomerates in the size range of 5 to 50 μm. Further analysis of particle size by means of a Malvern mastersizer confirmed the original zeolite crystal agglomerate powder to have an average particle size of 34 μm (Table 5.2). During the preparation of the catalyst washcoat suspension, these large particle agglomerates are partially reduced in size to an average particle size of approximately 14 μm, presumably as a result of attrition during the agitation process. The effect of zeolite particle size on suspension and coating properties is presented in Section 5.2.1.

5.1.2. Coating morphology

The SEM images of the directly-substituted zeolite washcoating and the original zeolite powder are compared in Figure 5.1. This shows that the washcoating has the same distinctive zeolite crystal agglomerate morphology as the original powder which tends to suggest that the zeolite morphology is dependant on the zeolite crystal agglomerate size used to prepare the washcoating. Figure 5.2 compares zeolite coatings prepared by the above washcoating method and the direct synthesis method (de la Iglesia et al., 2007), respectively. The coatings show a significant resemblance in terms of coating uniformity and surface roughness, despite previous claims that the washcoating yields an unsatisfactory uniformity (Wan et al., 2001).

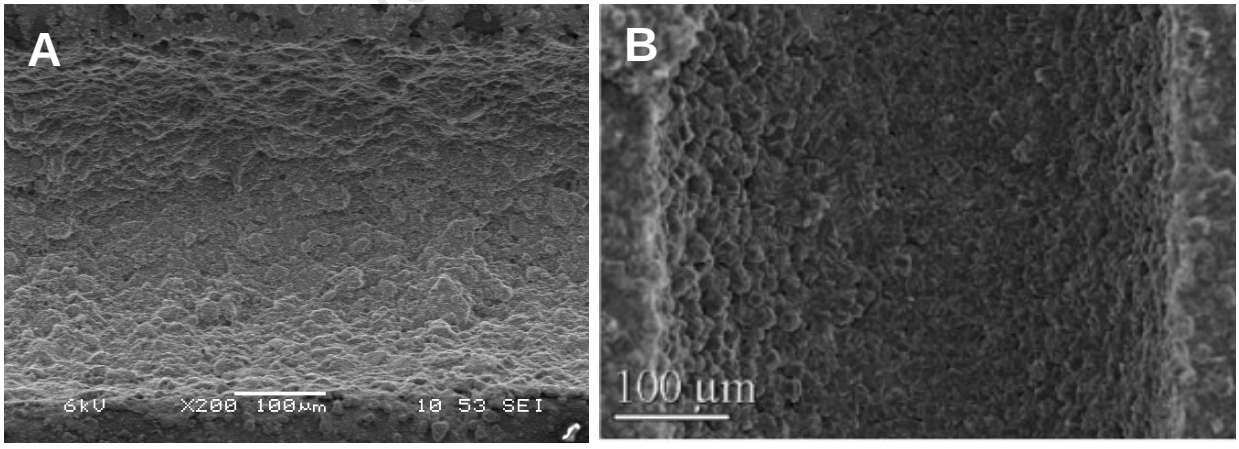

Figure 5.2: SEM image of (a). directly-substituted zeolite washcoating as per Figure 5.1 (b). ZSM-5 direct synthesis coating (de la Iglesia et al., 2007).

5.1.3. Zeolite crystal structure

In order to determine whether any significant structural change in the zeolite crystallites of the washcoat occurred due to calcination at 600˚C or from any other of the washcoating steps, XRD patterns and BET surface area analysis of the original zeolite crystal agglomerate powder and the directly-substituted washcoat powder were compared.

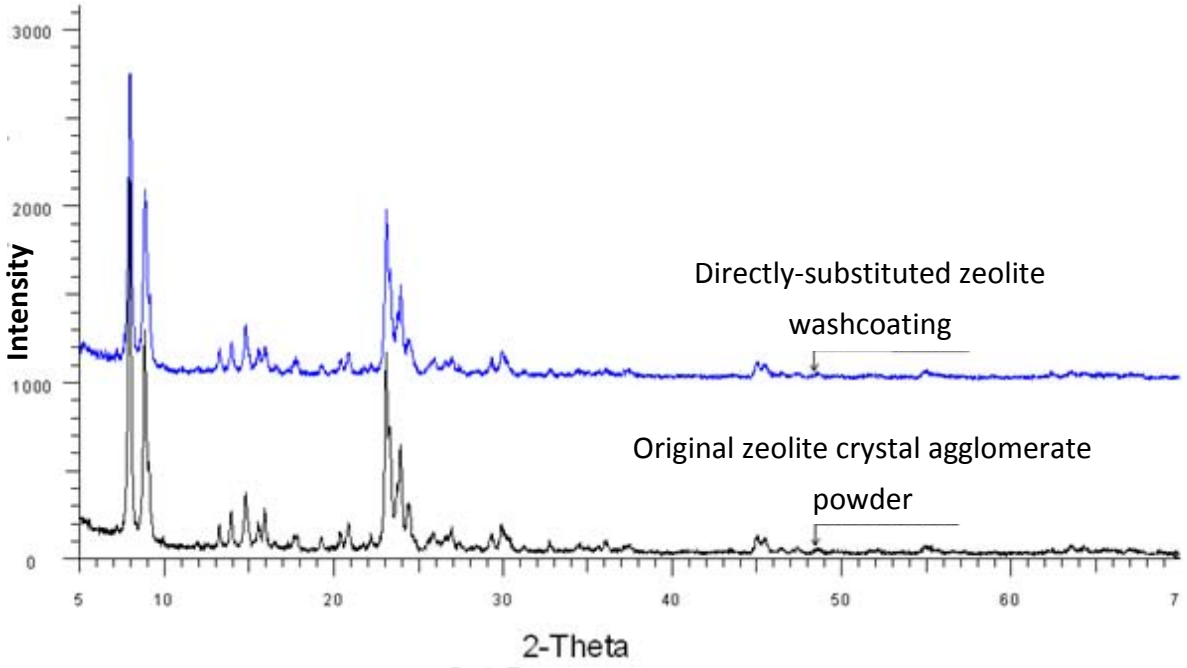

Figure 5.3: XRD patterns of calcined original zeolite crystal agglomerate powder and directly-substituted zeolite washcoat powder.

The XRD patterns showed comparable half height peak widths for both the original zeolite crystal agglomerate and the directly-substituted zeolite washcoat (Figure 5.3). Similarly, the BET surface area results showed no significant difference (Table 5.2), indicating that the crystal structure and size of the directly-substituted zeolite washcoat is not affected to any significant extent as a consequence of the washcoating preparation.

5.1.4. Suspension rheology

The zeolite suspension viscosity and pH are measured in order to evaluate the stability of the suspension. The suspension viscosity is measured with respect to shear rate (Figure 5.4) and ageing time (Figure 5.5), and the pH with respect to suspension ageing time (Figure 5.5).

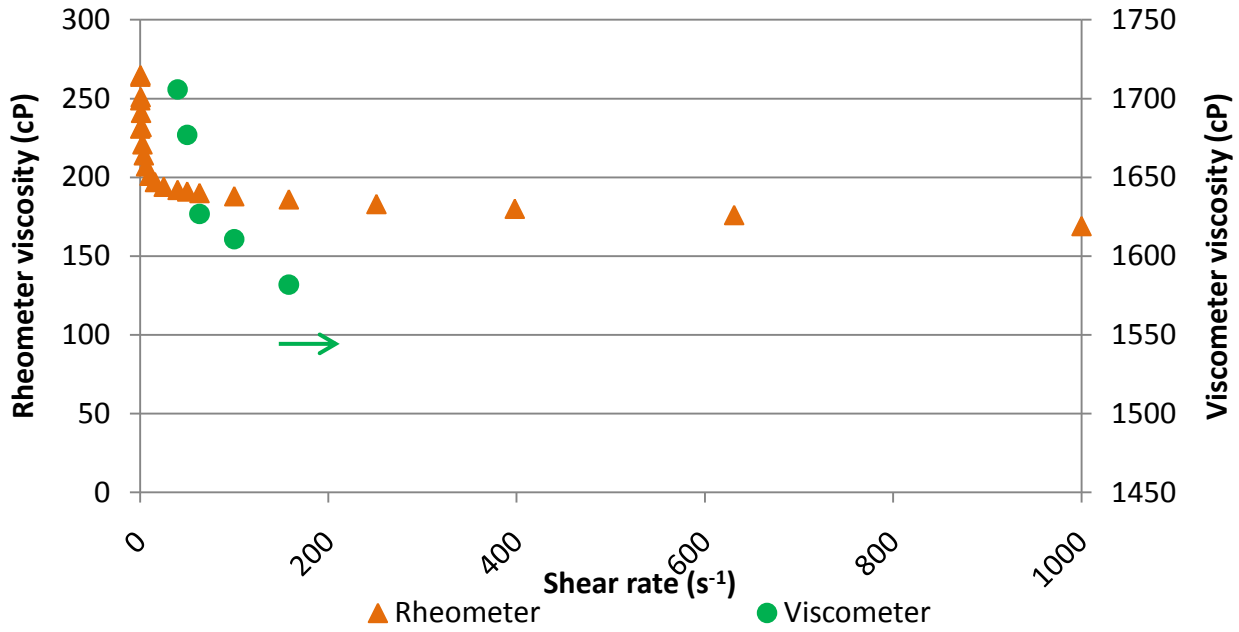

Figure 5.4: Viscosity of directly-substituted zeolite suspension versus shear rate measured using a rheometer and a viscometer.

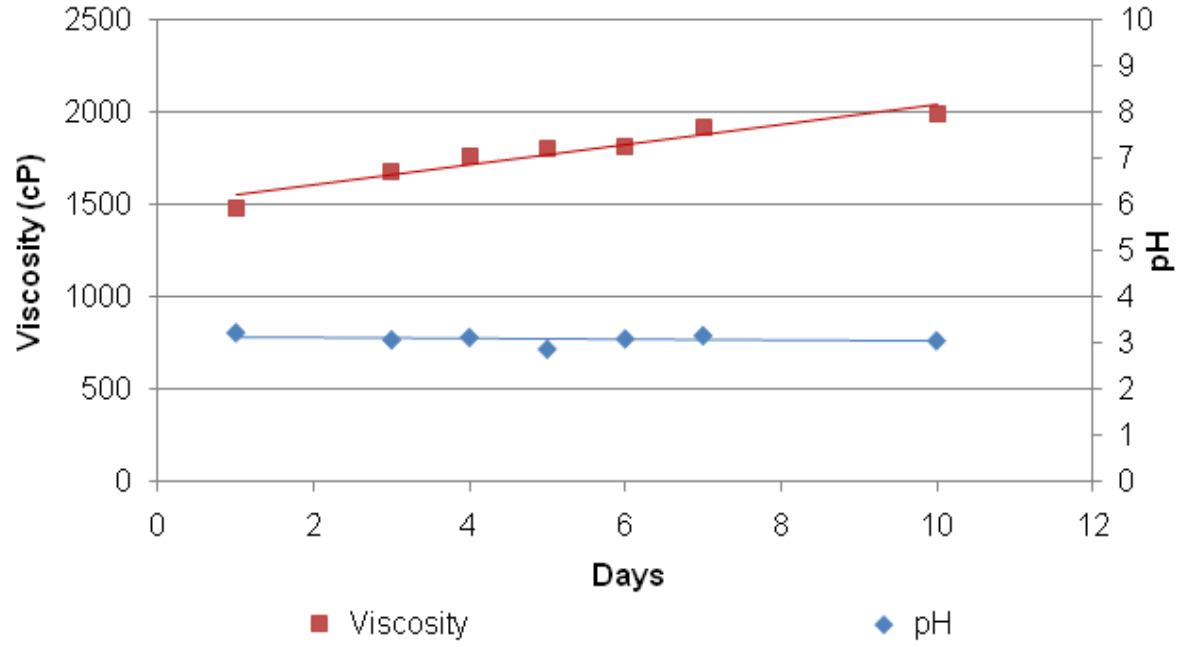

Figure 5.5: Directly-substituted zeolite suspension viscosity at a shear rate of 50 s^{-1} and pH with respect to number of days aged (stirred).

The viscosity of the directly-substituted zeolite suspension was evaluated using both a rheometer and viscometer, with the rheometer being applied to observe the viscosity over a wider range of shear rates (Figure 5.4). The viscosity was shown to decrease with increasing shear rate although the magnitude of the viscosity measurements differed substantially between the two methods. The viscometer was thought to be the least accurate since the viscometer reading was dependant on more external variables (Section 4.4.2). The rheometer was, however, not available for experimentation (used in training at IMM).

The suspension viscosity decreases with increasing shear rate which indicates a pseudo-plastic or shear-thinning behavior which is characteristic of suspensions which flocculate and do not disperse well (Vallar et al., 1999). This same pseudo-plastic behavior was reported for a washcoating suspension containing ZSM-5, water and colloidal silica for viscosities of 3.3 - 2000 cP, shear rates up to 200 s^{-1} and solid concentrations between 20 and 40% (Mitra et al., 2008).

The effect of ageing time on suspension viscosity (Figure 5.5) shows that with increasing ageing time, the suspension viscosity increases, indicating that the zeolite suspension is relatively unstable. Moreover, this strong dependency of suspension viscosity on ageing time affects suspension reproducibility and reusability, as well as final coating properties (Section 5.2.3.).

The pH remained relatively constant at an average pH of 3.2 (Figure 5.5) indicating no significant changes to the suspension's surface charges with respect to ageing time and, consequently, this property was not further investigated in this study.

5.1.5. Adhesion

The directly-substituted zeolite washcoating exhibits a catalyst weight loss of 8.1% after the drop test. In order to gain a qualitative understanding of the zeolite washcoat adherence, a directly-substituted zeolite coated test plate before and after the drop test is shown in Figure 5.6, clearly indicating the washcoat spalling. So as to improve zeolite washcoat adhesion, the suspension properties were further evaluated (Section 5.2).

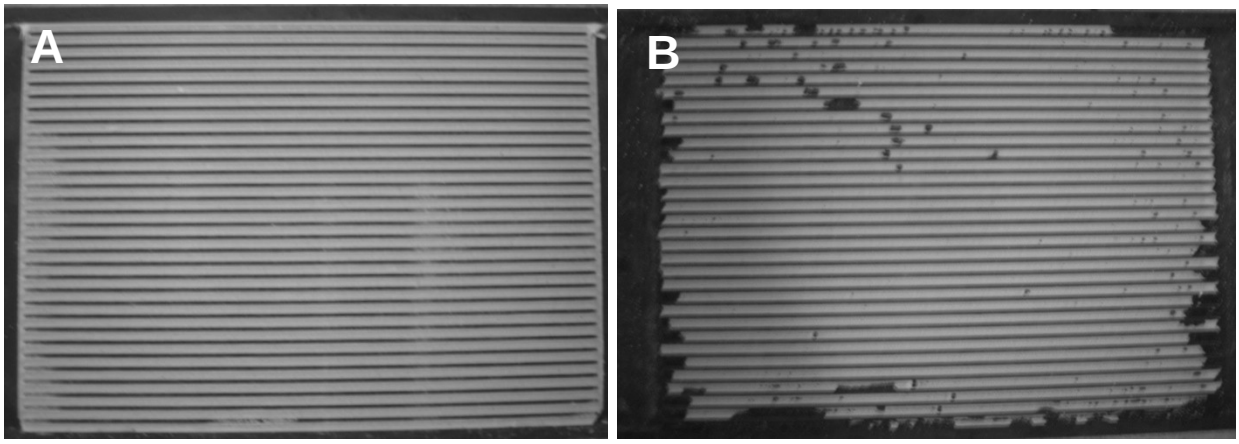

Figure 5.6: SEM images of a directly-substituted zeolite coated microchannel test plate (a) before adherence drop test and (b) after adherence drop test.

5.1.6. Catalyst loading

The amount of catalyst coated onto the test plate is 0.0430 g which translates to 0.3 mg/cm^2 when taking into account the surface area of the microchannels (Appendix A.3) on the test plate.

During the drying and calcination process, water and other organic additives are removed leaving behind the inorganic solids. The solids concentration will affect the amount of solids left behind after the drying and calcination stages, whilst the channel geometry will affect the amount of washcoating suspension deposited. The effect which the channel dimensions have on coating properties is presented in Section 5.7.

By taking into account the total volume of the microchannels, the theoretical catalyst loading can be calculated based on the solids concentration (Appendix A). For the particular plate (Plate B) and solids concentration of this experiment, the theoretical catalyst loading ranges between 0.0314 g and 0.0452 g (variation due to different channel depth and width) whilst the actual catalyst loading gives a comparable result (0.0430 g).

5.2. Suspension properties and modifications

In order to improve the coating suspension and final washcoat properties, various modifications to the directly-substituted suspension previously presented in Section 5.1 were evaluated. Principally, the effects of the main suspension properties such as particle size, suspension composition, viscosity, and ageing time were investigated.

5.2.1. Reduction of zeolite particle size

5.2.1.1. Zeolite milling

To evaluate the effect of zeolite particle size on coating properties, the particle size of the original zeolite crystal agglomerate powder was reduced by micronizing with isopropanol as the solvent (Section 4.1.1.2). The milling time was adjusted to give various particle size fractions as illustrated in Figure 5.7.

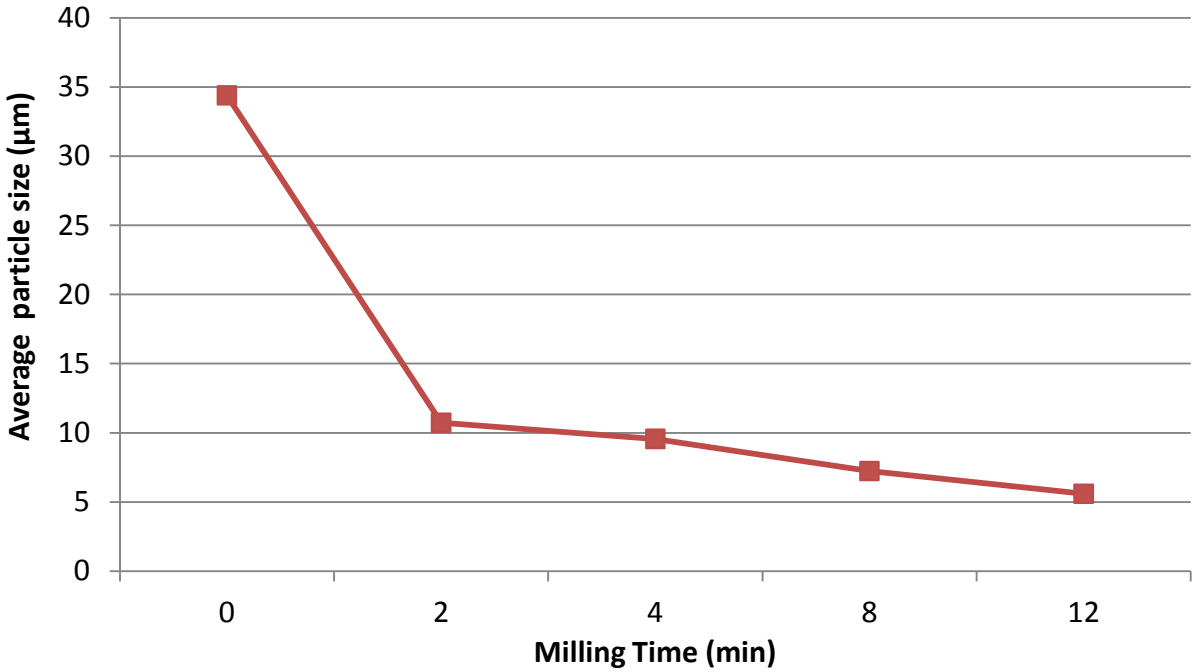

Figure 5.7: Average particle size of H-MFI-90 zeolite catalyst after milling for various times.

Figure 5.7 indicates a significant reduction of zeolite catalyst particle size for milling times up to 2 minutes, and smaller changes in particle size when prolonging the milling time.

5.2.1.2. Effect of milling on physical properties of zeolite powder

To assess whether the milled powder had undergone any structural changes from the milling process, XRD patterns and BET surface areas were compared to the original zeolite powder. The results are shown in Figure 5.8 and Table 5.3. Additionally, the adherence properties of washcoats prepared from the milled zeolite powder, are presented in Table 5.3.

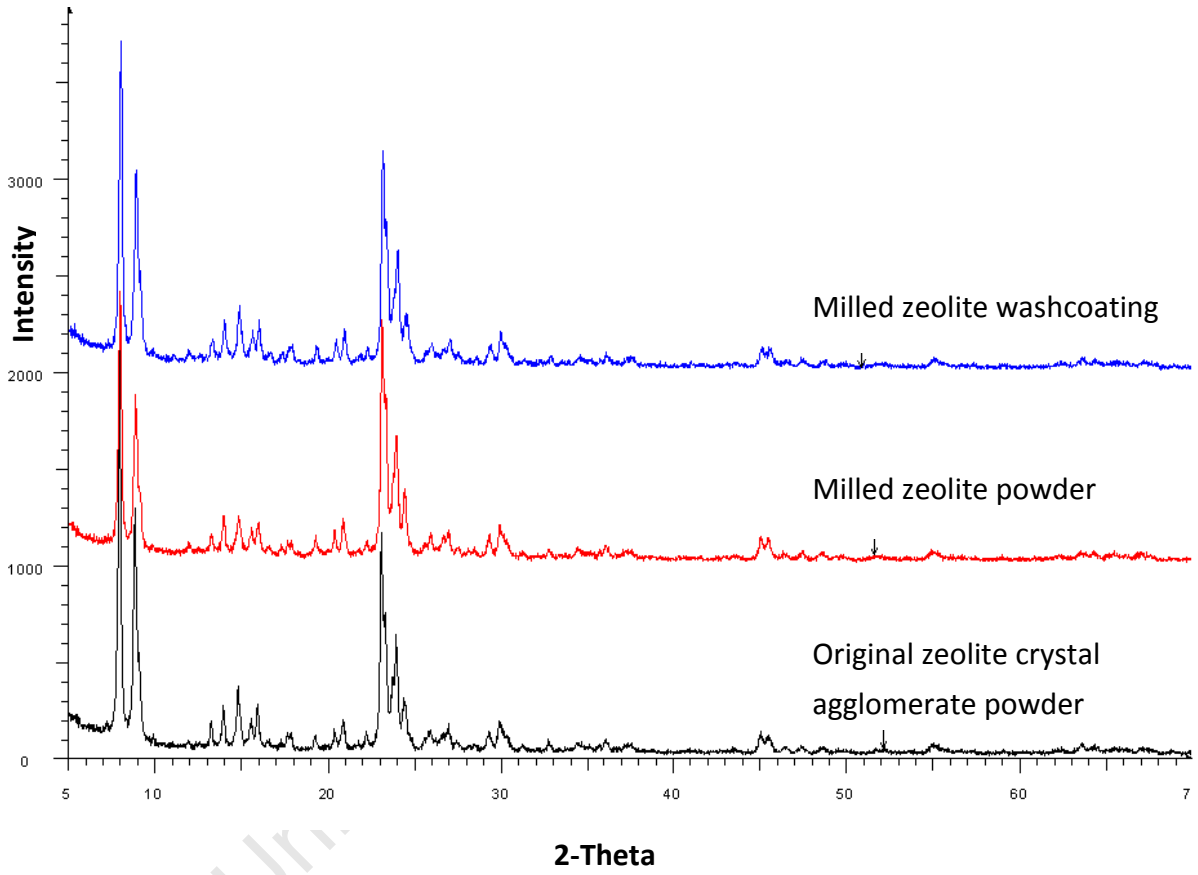

Figure 5.8: XRD patterns of milled zeolite washcoating, (7 µm) milled zeolite powder, and original (34 µm) zeolite crystal agglomerate powder.

Table 5.3: Comparison of zeolite powder before and after thermal treatment at 600 ˚C.

	Particle size [a] (µm)	BET Surface Area ($m^2.g^{-1}$)	Powder colour	Adherence test [b] (wt% lost)
Milled powder before calcination	7	276	brown	4.1
Milled powder after calcination	7	376	white	1.3

[a] *Average particle size of zeolite powder*
[b] *Percentage mass loss of catalyst after drop tests.*

The XRD patterns of the milled zeolite powder before and after milling, as well as the milled zeolite washcoating, did not show any significant changes in the zeolite structural properties. However, the BET surface area of the milled zeolite powder before calcination was lower (276 $m^2.g^{-1}$) than that of the original zeolite crystal agglomerate powder (369 $m^2.g^{-1}$). This may be attributed to the formation of 'coke' from the isopropanol milling solvent in the presence of the zeolite catalyst, a phenomena supported by the observed brown colour of the catalysts. Subsequent thermal treatment in air according to the same 600 °C temperature programme used for calcining the washcoat (Section 4.3.5) resulted in a milled powder of a white colour and a BET surface area (376 $m^2.g^{-1}$), comparable to the original zeolite crystal agglomerate powder. Consequently, the BET findings further confirm the absence of any structural degradation of the zeolite catalyst during milling.

The use of the milled powder, before thermal treatment, for washcoating resulted in washcoats of poor physical adherence. The suspension and coating results of the zeolite powder after thermal treatment is given in the subsequent section. In contrast, washcoats prepared from milled zeolite powders after calcination were of a good quality as described in Section 5.2.1.3.

5.2.1.3. Effect of reduced zeolite particle size on coating and suspension properties

Zeolite washcoat suspensions containing the smaller particle size powder (after 600 °C thermal treatment) were prepared and coated onto the microchannel plates to give the coating properties summarized in Table 5.4 and Figure 5.9b.

Table 5.4: Properties of H-MFI-90 zeolite washcoating and suspension with reduced particle size after thermal treatment.

	Milling time (min)	Zeolite particle size [a] (µm)	Adherence test [b] (wt% lost)	Viscosity (cP at 50 s^{-1})
Directly-substituted washcoat (Section 5.1)	0	34	8.1	1677
Zeolite - A	2	10	2.4	957
Zeolite - B	8	7	1.3	758

[a] *Average particle size of zeolite powder*
[b] *Percentage mass loss of catalyst after drop tests.*

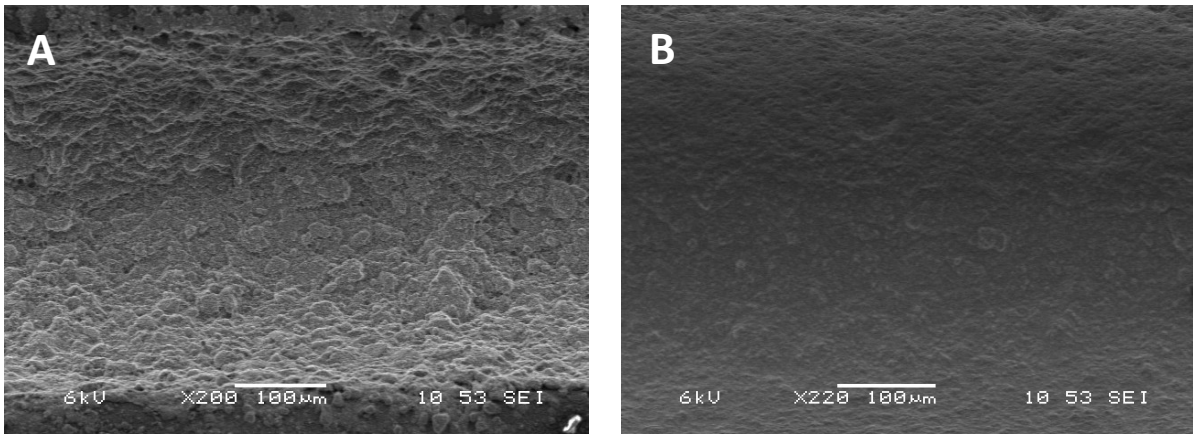

Figure 5.9: SEM images of: (a) Directly-substituted zeolite washcoat (b) Zeolite - B, 7 µm zeolite washcoat.

With increasing milling time and associated decrease in average particle size, a decreased suspension viscosity and increased washcoat adherence are observed (Table 5.4). Similarly, Agrafiotis et al. (2000a) found that a smaller solid particle size in the suspension improved the adhesion onto stainless steel supports and ascribed this as being due to anchorage and interlocking of the particles with small size.

Figure 5.9 illustrates the microchannel plate washcoat morphology for the original zeolite crystal agglomerate powder (34 µm) and the reduced zeolite particle size (7 µm) coatings. The original zeolite coating (Figure 5.9a) had a rougher surface morphology probably caused by the larger zeolite crystal agglomerate particles, whereas the coating prepared from smaller zeolite particles (Figure 5.9b) exhibits a smoother coating surface. A smaller particle size thus appears to permit the formation of a tighter particle packing that, in turn, results in a smoother surface and better adhesion whereas the larger zeolite particle size seems to cause a looser particle packing resulting in a less adherent and rougher surface coating.

5.2.2. Suspension composition: Inorganic binder addition

The influence of the addition of an inorganic binder to the zeolite suspension was evaluated by considering two binders, namely, colloidal silica and γ-Al_2O_3.

5.2.2.1. Addition of colloidal silica binder

Colloidal silica has been widely used as a binder for zeolite washcoating of monoliths and was therefore attempted for use to improve adherence of the microchannel washcoats, prepared with the original zeolite powder (d_p^{ave} = 34 µm) (Beers et al., 2003; Zamaro et al., 2005; Mitra et al., 2008; Eleta et al., 2009; Lisi et al., 2009). Table 5.5 presents the properties of silica containing suspensions and washcoats.

Table 5.5: Suspension composition and properties of washcoatings containing colloidal silica as binder.

Suspension [a]	PVA (g)	Silica (g)	Adherence test [b] (wt% catalyst lost)	Viscosity (cP of 50 s^{-1})
Silica A	2.5	2.5	*	*
Silica B	0	2.5	*	*
Silica C	1.25	1.25	63.2	696

[a] Zeolite: 10 g, Acetic acid: 0.5 g, Distilled water: 37.5 g
** Reading not taken due to the formation of a thick viscous gel-like suspension*
[b] Percentage mass loss of catalyst after drop tests.

The addition of 2.5 g PVA and 2.5 g silica in the "Silica A" suspension resulted in a highly viscous gel-like suspension to form. To reduce the suspension viscosity, no PVA was added to the "Silica B" suspension which resulted in a lower suspension viscosity but which was still too high to measure using a viscometer. Reducing the amount of colloidal silica to 1.25 g, together with the addition of 1.25 g of PVA, yielded a suspension viscosity which was adequate but nonetheless a washcoat suspension which resulted in a poor adherence (63.2% catalyst lost). The poor adherence of the colloidal silica containing washcoat may possibly be attributed to the general washcoating methodology whereas, for monolith washcoating, a more viscous suspension is required to allow for sufficient catalyst loading. In the microchannel washcoating method, a suspension which is too viscous results in a non-uniform coating which, in turn, will affect adherence (Section 5.2.3).

5.2.2.2. Addition of γ-Al_2O_3 binder

Previously, the addition of Al_2O_3 has been used as a binder to improve the strength of the resulting zeolite extrudates (Kasture et al., 2007). Moreover, the washcoating of γ-Al_2O_3 has also resulted in coatings with good adherence (Zapf et al., 2006). Consequently, a colloidal γ-

Al_2O_3 powder of 3 µm particle size was chosen as a binder additive to the original zeolite crystal agglomerate powder (d_p^{ave} = 34 µm) formulations.

In order to evaluate the influence of the γ-Al_2O_3 binder, various zeolite:γ-Al_2O_3 ratios were employed, in all cases keeping the total solids concentration constant as the latter influences the final coating thickness and solids loading. Table 5.6 summarises the properties of the suspensions containing γ-Al_2O_3 and the resulting calcined washcoats whilst SEM images of the corresponding coatings are presented in Figure 5.10.

Table 5.6: Washcoat and suspension properties for various ratios of H-MFI-90 zeolite and γ-Al_2O_3.

Suspension	Zeolite (g)	γ-Al_2O_3 (g)	Adherence test[a] (wt% lost)	Viscosity (cP of 50 s^{-1})	Average particle size (µm)	Cat. loading (g)	BET Surface area ($m^2.g^{-1}$)
Zeolite 100%	10	-	8.1	1677	34	0.0430	365
Zeolite 90%	9	1	6.2	991	31[b]	0.0429	332
Zeolite 85%	8.5	1.5	1.7	875	30[b]	0.0426	313
Zeolite 75%	7.5	2.5	1.6	748	26[b]	0.0450	281
Zeolite 50%	5	5	0.9	614	19[b]	0.0438	209
Alumina	-	10	0.3	437	3	0.0587	67

[a] *Percentage mass loss of catalyst after drop tests*
[b] *The particle size of these mixed powders is estimated as a weighted average particle size of the original zeolite crystal agglomerate powder (34 µm) and γ-Al_2O_3 powder (3 µm).*

It may be seen from Table 5.6 that an increase in γ-Al_2O_3 composition improves the adherence of the washcoat on the microchannel plates. This improvement in adherence may be attributed to the γ-Al_2O_3 having a lower particle size and hence reducing the average particle size, as well as decreasing the suspension viscosity. Likewise, the SEM images in Figure 5.10, show that with increasing γ-Al_2O_3 content, the coating morphology becomes smoother which may also be attributed to the smaller γ-Al_2O_3 particle size enabling a tighter particle packing between the larger zeolite particles. This tighter packing results in better anchorage and interlocking of the suspension particles and consequently, in a better coating adherence which is similar to the effect observed for reduced zeolite particle size in Section 5.2.1.

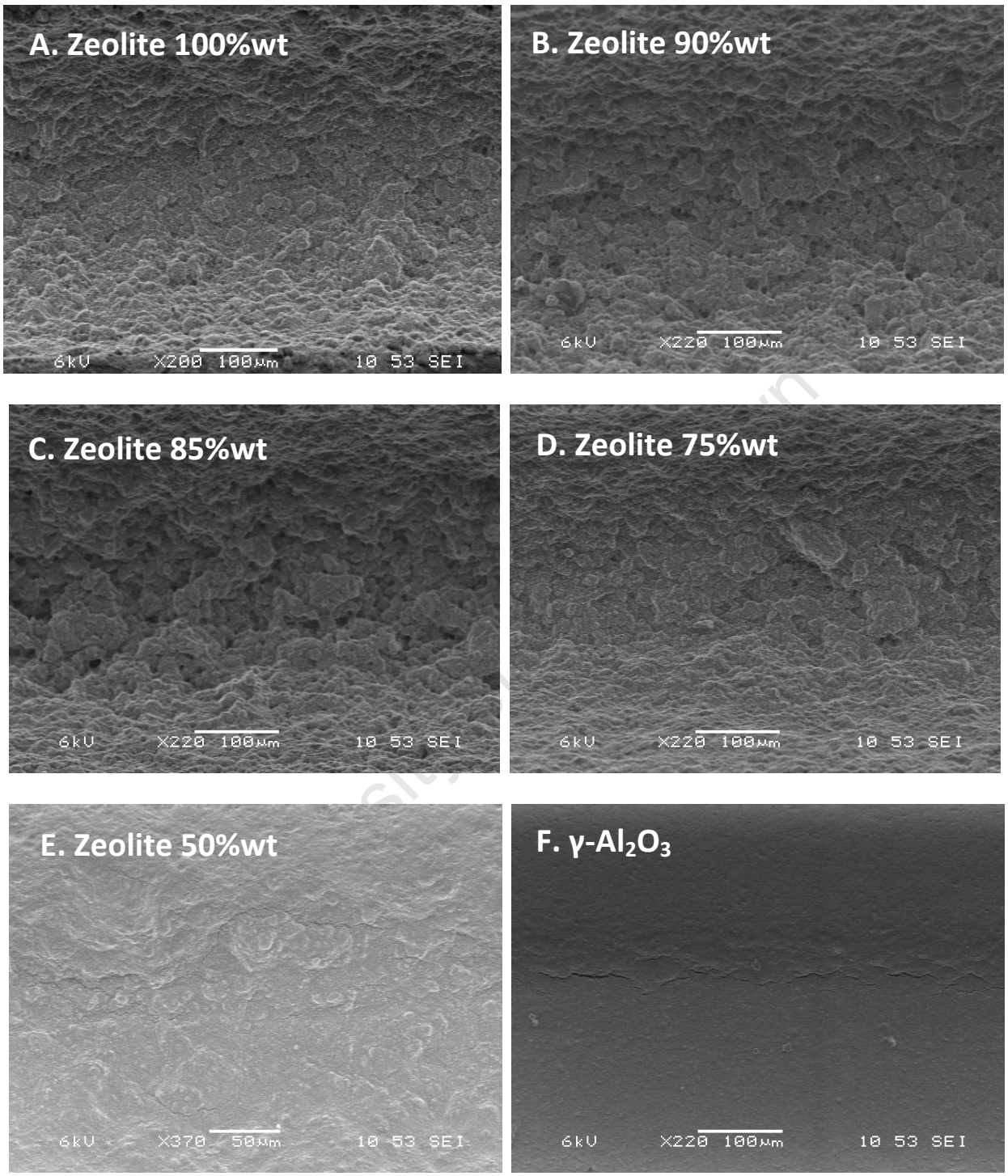

Figure 5.10: SEM images of H-MFI-90 zeolite (d_p^{ave} = 34 µm) washcoatings containing various amounts of alumina (a) 100 wt % zeolite , (b) 90 wt% Zeolite, (c) 85 wt % Zeolite, (d) 75 wt % Zeolite and (e) 50 wt % Zeolite, and (f) 100 wt% γ-Al_2O_3.

A further effect which the addition of γ-Al_2O_3 has on the suspension viscosity is depicted in Figure 5.11, where viscosity is plotted with respect to ageing time for suspensions containing different ratios of γ-Al_2O_3 and zeolite crystal agglomerate powder.

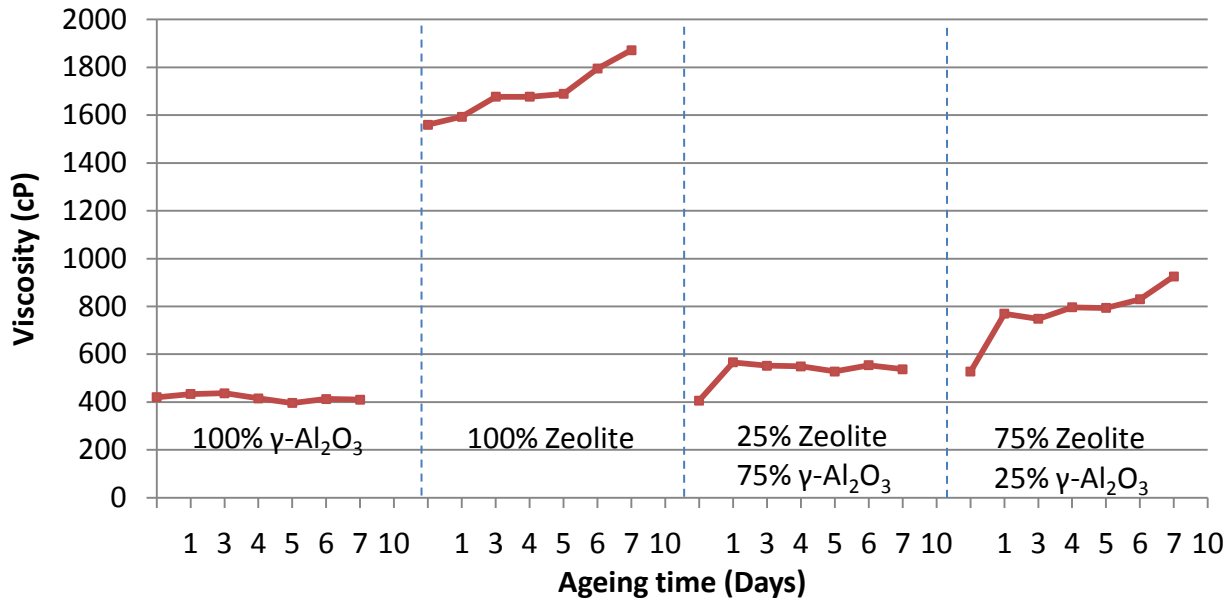

Figure 5.11: The effect of ageing time and addition of γ-Al_2O_3 binder on suspension viscosity.

The addition of γ-Al_2O_3 lowers the viscosity (Table 5.6) and stabilizes the suspension (Figure 5.11). As shown in Section 5.1.4, the directly-substituted zeolite suspension exhibits a pseudo-plastic rheology and a viscosity which increases with ageing time. In Figure 5.11, the 100% γ-Al_2O_3 suspension is, by comparison, far more stable with a relatively constant and lower viscosity with the suspensions of intermediate composition showing intermediate rheological properties between the 100% γ-Al_2O_3 and 100% zeolite end-points. The addition of γ-Al_2O_3 binder is, therefore, beneficial to the stability of the washcoating suspension, a property which aids in reproducibility of suspension preparation.

The presence of γ-Al_2O_3 in the washcoat comes, however, at the expense of zeolite catalyst and, consequently, the amount of γ-Al_2O_3 needs to be minimized. The XRD patterns showed no significant structural changes when γ-Al_2O_3 was added between 0 and 25 wt% γ-Al_2O_3 content, whereas, for suspensions containing 50% γ-Al_2O_3 or more, the XRD patterns clearly reflect a reduction in the diffraction intensities which is due to zeolite dilution by the presence of the amorphous γ-Al_2O_3 (Figure 5.12). The BET surface area of γ-Al_2O_3 is also lower than the zeolite

crystal agglomerate powder which results in the coatings of lower surface area depending on the quantity of γ-Al_2O_3 added. A high amount of γ-Al_2O_3 will improve the adherence, coating morphology and suspension stability, but will in turn reduce the amount of zeolite coated and hence the activity and lower the catalyst surface area.

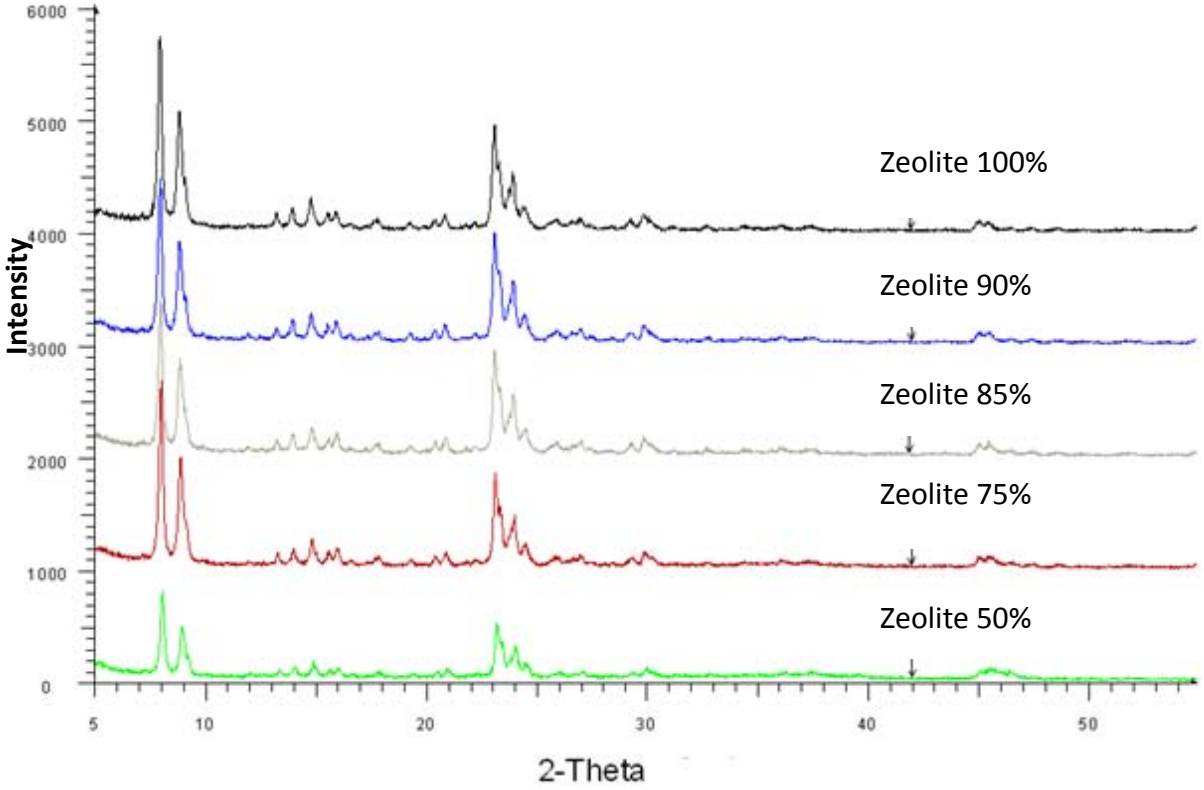

Figure 5.12: XRD patterns of H-MFI-90 zeolite powder washcoats containing varying amounts of γ-Al_2O_3.

5.2.3. Suspension viscosity

Up to this point, the effect which the suspension viscosity has on the coating adherence has not been evaluated in detail due to it being dependant on other suspension variables such as particle size, binder addition, and ageing time. To ascertain whether the suspension viscosity affects the coating adherence, various different suspension compositions were used as a basis for comparison (Figure 5.13).

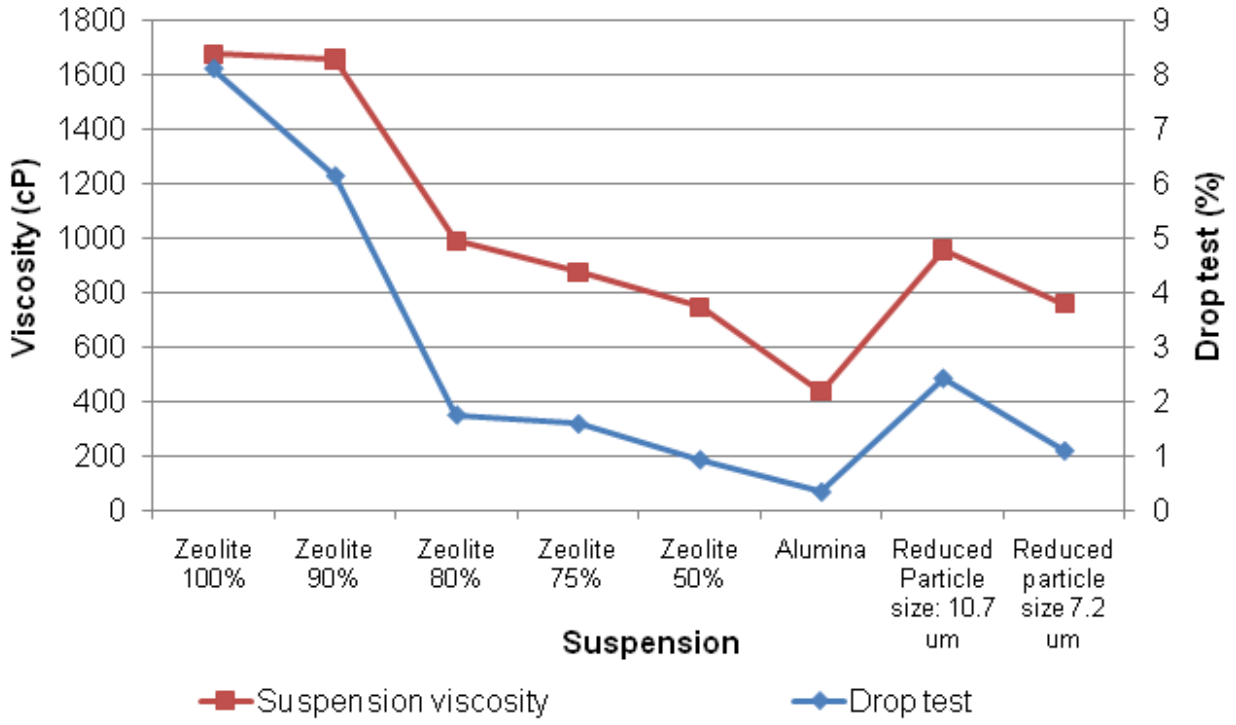

Figure 5.13: Effect of suspension viscosity on coating adherence.

Figure 5.13 indicates the trends in suspension viscosity and washcoat adherence as a function of washcoat composition, material (zeolite vs. γ-Al_2O_3) and particle size to be remarkably similar. As the suspension viscosity decreases, the amount of catalyst lost in the drop test decreases thus indicating an improvement in adherence. A possible connection for the relationship between suspension viscosity and washcoat adherence may be gained from an observation of the final washcoat. A cross-sectional image of a microchannel coated with a 75% zeolite washcoat (Figure 5.14) shows the microchannel walls to have a slightly thicker coating (38 – 46 µm) in comparison to the bottom of the microchannel (30 µm), a finding which may be attributed to the viscosity of the suspension (Germani et al., 2007). On the other hand, Figure 5.15 shows a Zeolite 75% coating after the drop test where damage (material loss) seems mostly to occur on the walls of the microchannels, where the coating is thickest. Consequently, decreasing the suspension viscosity so as to improve the coating uniformity may improve adherence. Note should, however, be made of the poor suspension stability and higher viscosity of zeolite-rich suspensions elsewhere in this report.

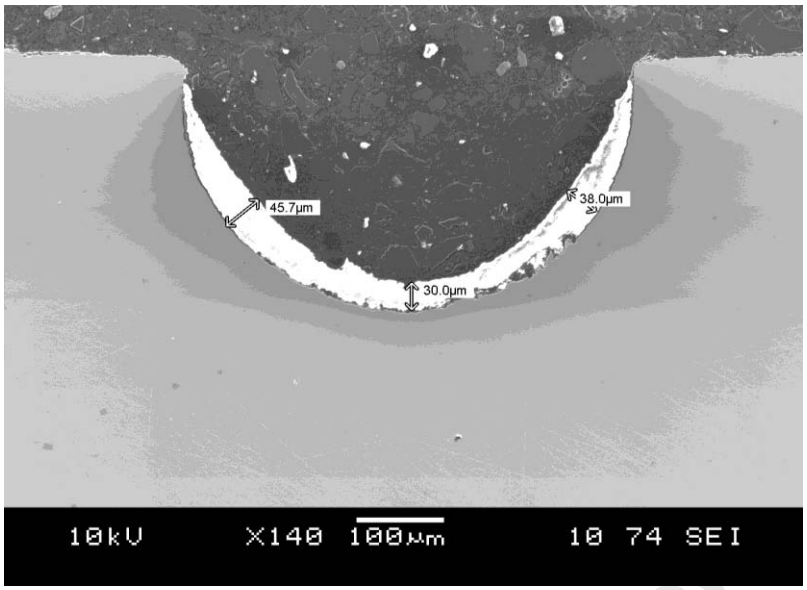

Figure 5.14: SEM image of cross sectional view of microchannel coated with 75 wt% Zeolite and 25 wt% γ-Al_2O_3 washcoating.

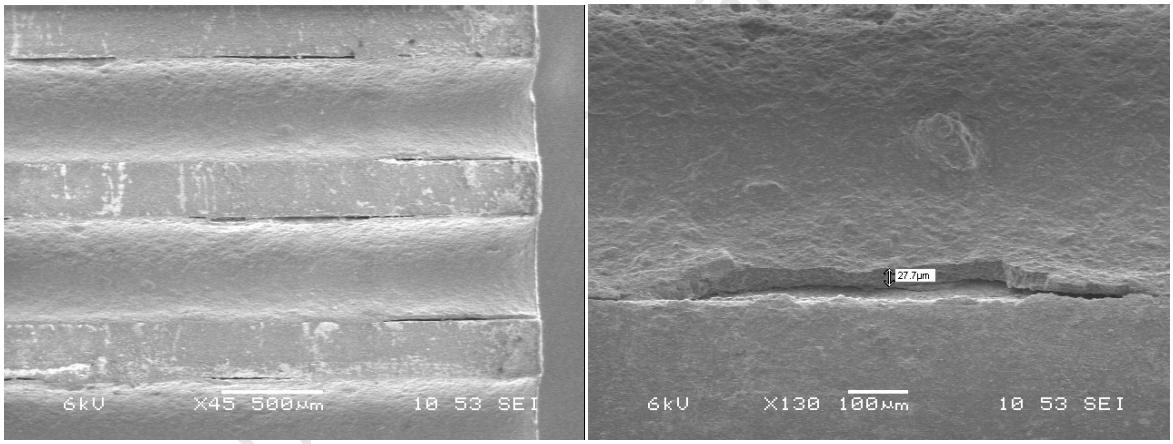

Figure 5.15: SEM images of 75 wt% Zeolite washcoating after drop test.

5.3. Optimization of zeolite coating

To incorporate the benefits of both the reduction of zeolite powder particle size (Section 5.2.1), as well as the addition of γ-Al_2O_3 binder (Section 5.2.2), a combination of these influences was incorporated into the zeolite washcoating methodology. A suspension where the solids concentration comprised 75 wt% H-MFI-90 zeolite and 25 wt% γ-Al_2O_3 was used as a basis for a study considering, different zeolite particle sizes. Table 5.7 shows the washcoat suspension and calcined coating properties whilst Figure 5.16 depicts the SEM images of the respective coatings.

Table 5.7: Properties of the optimised washcoating and suspension containing 25% wt γ-Al_2O_3 and reduced zeolite particle size.

Suspension	Zeolite particle size[a] (µm)	Suspension particle size[b] (µm)	Viscosity (cP of 50 s^{-1})	Adhesion test[c] (wt% lost)	Catalyst loading (g)	BET SA ($m^2.g^{-1}$)
Zeolite 75% - A	16	8	1197	0.2	0.0444	282
Zeolite 75% - B	8	7	1017	0.1	0.0472	286

[a] *Average particle size of zeolite catalyst powder before synthesizing suspension*
[b] *Washcoat suspension particle size before coating determined by Malvern Mastersizer*
[c] *Percentage mass loss of catalyst after drop tests*

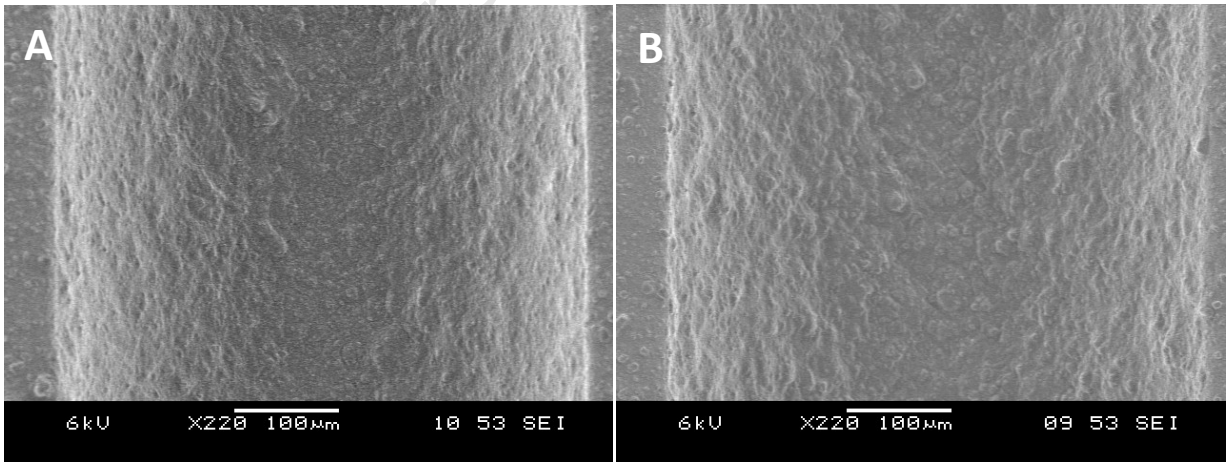

Figure 5.16: SEM images of optimized suspensions: (a) Zeolite 75% - A (particle size 16 µm); (b) Zeolite 75% - B (particle size 8 µm).

The use of γ-Al_2O_3 binder, together with the reduction of zeolite particle size, gave a coating which has a good adherence of below 0.5% weight loss after the drop test. Although the two suspensions have a different initial particle size of 16 µm and 8 µm, respectively, this difference in particle size becomes minimal after the suspensions have been stirred for 3 days. The larger particle agglomerates of both suspensions are reduced in size to a mean of approximately 7 µm. The SEM images (Figure 5.16) further show the coatings of the two suspensions to have similar morphology despite the initial differences in zeolite particle size. This is most probably due to the particle size of the final suspension being almost identical and which results in a similar particle packing in the coating.

The BET surface area of the optimised washcoatings is lower than the original zeolite powder due to the presence of the γ-Al_2O_3, however, it is essentially the same as that prepared with the original (as-received) zeolite agglomerate powder when applied as a 75 wt% zeolite mixture with γ-Al_2O_3 (Table 5.6). Even so, the viscosity of these suspensions is considerably higher than that observed in suspensions of a similar composition but having larger particle size (Table 5.6), an observation which may simply be an artifact of when the suspensions were prepared. This latter matter of reproducibility is presented in Section 5.6.

5.4. Further washcoat adherence testing

The adherence strength of the washcoated catalyst material onto the microchannel plates is critical as it will strongly influence the durability of the catalyst under the typically severe reaction conditions in the microchannel reactor. To further assess the adherence of the coating when in the presence of a liquid, the coated microchannel plates were subjected to an ultrasonification test in petroleum ether for an hour, followed by a further hour under ultrasonification in isopropanol. The second ultrasonic treatment is simply to determine whether the coating will be adversely affected by the isopropanol reagent when conducting the test reaction in the microchannel reactor. Figure 5.17 illustrates the percentage catalyst mass lost for the various adhesion tests.

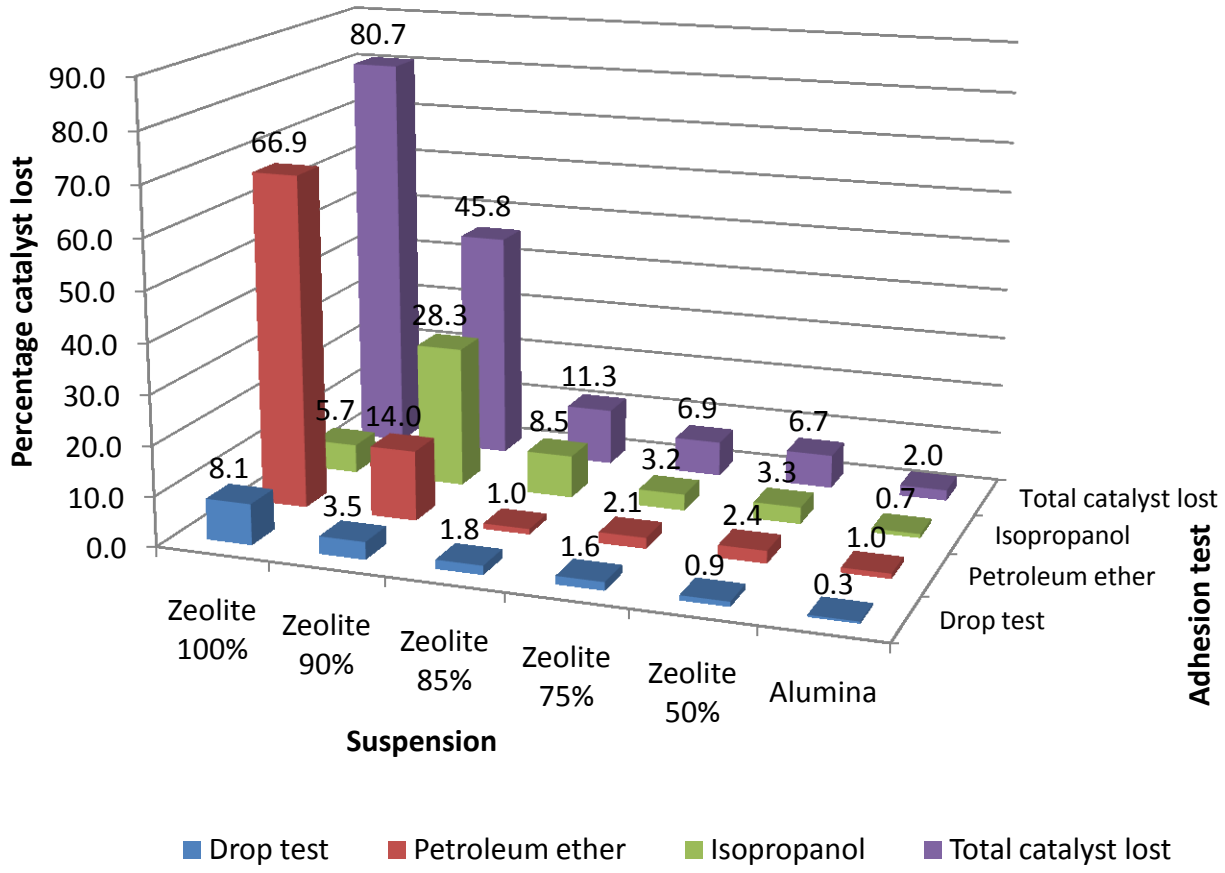

Figure 5.17: Percentage catalyst lost after various adhesion tests with varying concentrations of alumina suspension coatings.

In general, the ultrasonification tests indicated a greater percentage catalyst mass loss when compared to the drop test, however, with the same trend of increasing γ-Al_2O_3 content corresponding to an improvement in the coating adherence. According to Stefanescu et al. (2007), a weight loss below 10% for an hour ultrasonification in petroleum ether is considered a stable coating. Washcoatings containing more than 10% γ-Al_2O_3 are therefore considered stable in this study.

The 100% Zeolite coating had a poor adherence with some 80% of the catalyst lost after the adherence testing. Due to the poor adherence of this coating, most of the catalyst is lost in the first ultrasonification treatment using petroleum ether as solvent. The smaller percentage of catalyst lost in the isopropanol ultrasonification is due to there being less catalyst coating left on the plate.

For the other suspensions, the greatest amount of catalyst was lost in the second ultrasonification treatment using isopropanol as solvent, however, it is considered that this finding is mostly due to the time of ultrasonification rather than the nature of solvent used. Nonetheless, it should be noted that the use of water as a solvent for ultrasonification resulted in a substantially higher loss of catalyst for all suspensions. The exact reason for this is unknown.

5.5. Washcoat properties after chemical reaction

Further evaluation of the washcoat adherence was done by visually comparing the zeolite washcoat after thymol synthesis to the fresh zeolite washcoat (Figure 5.18) and by means of elemental analysis in Table 5.8. A single microchannel washcoat is presented visually after thymol synthesis in Figure 5.19 and centre and outer channels are compared visually after the thymol synthesis in Figure 5.20.

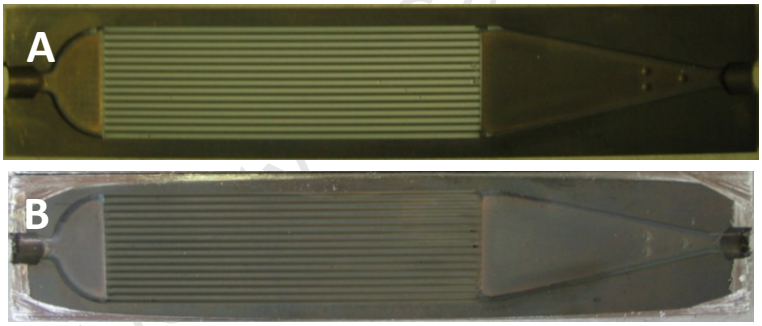

Figure 5.18: Microchannel reactor plates with zeolite washcoat (75 wt% Zeolite (d_p^{ave} = 34 µm) , 25 wt% γ-Al_2O_3): a) before, and b) after thymol synthesis.

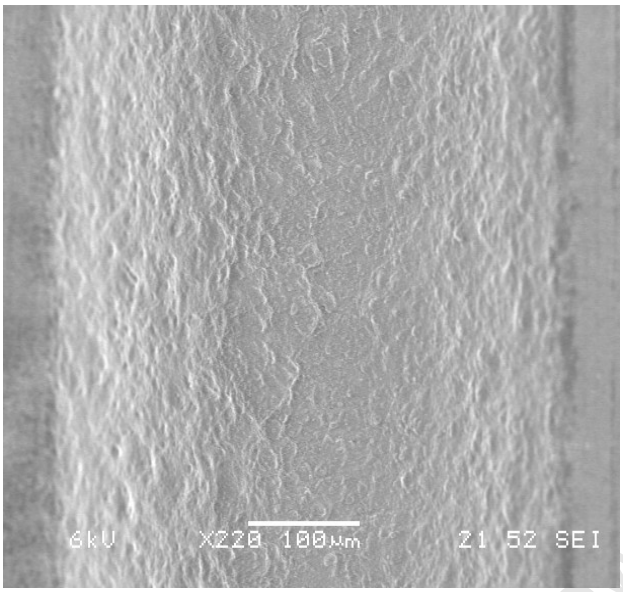

Figure 5.19: Single channel of microchannel reactor plate with zeolite washcoat after thymol synthesis (75 wt% Zeolite (d_p^{ave} = 34 µm), 25 wt% γ-Al_2O_3).

Table 5.8: SEM EDX analysis of coating before and after thymol synthesis.

Coating	C (wt %)	Si (wt %)	Al (wt %)	O (wt %)
Before reaction	2	52	23	24
After reaction	9	46	20	25
After reaction and calcination (600˚C)	4	48	22	26

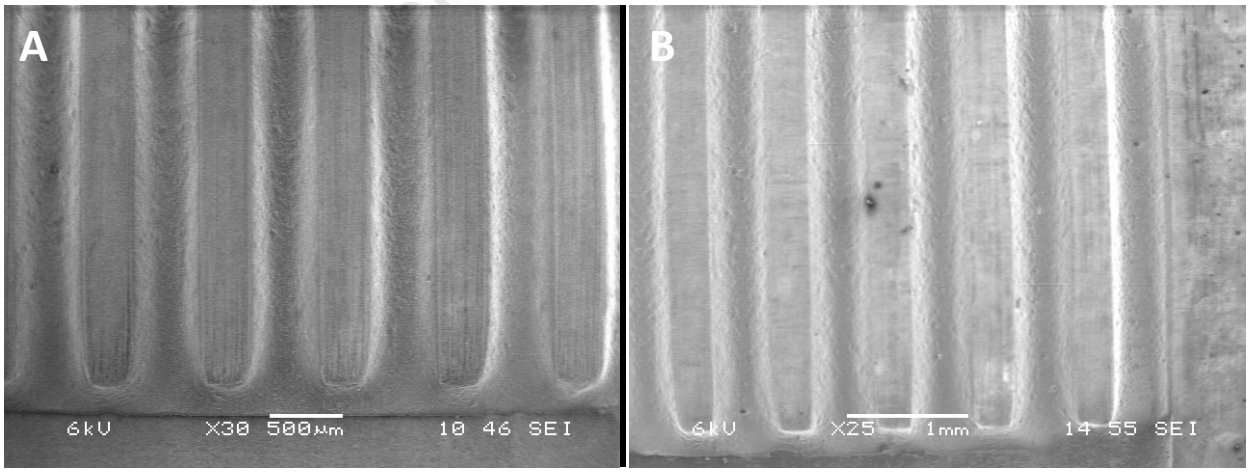

Figure 5.20: Microchannel reactor plates with zeolite washcoat (75 wt% Zeolite (d_p^{ave} = 34 µm), 25 wt% γ-Al_2O_3) after thymol synthesis (a) centre microchannels (b) outer microchannels.

After the test reaction, the zeolite washcoat is noticeably a darker colour which is attributed to the formation of 'coke' on the zeolite during the thymol synthesis reaction (Figure 5.18), a finding which confirmed by the elemental analysis data of Table 5.8. Calcination of the spent plates at 600˚C yields a washcoat similar in appearance to the original white colour and SEM EDX confirms a decline in the carbon content in the coating (Table 5.8). A similar discolouration was observed with all the spent catalysts from fixed-bed reactor testing suggesting that catalyst coking is the dominant deactivation process in all experiments of this study.

After the test reaction, the washcoat also shows no visible loss of material when comparing the microchannel reactor plates (Figure 5.18). A more detailed view of a single channel washcoat after the test reaction (Figure 5.19) further indicates no change in the washcoat morphology, also confirming the integrity of the zeolite washcoat. It should be noted that the zeolite crystal agglomerate powder particle size was not reduced. The good adherence of the Zeolite 75% washcoating observed in the test reaction indicates that although the zeolite particle crystal agglomerates were not milled, the adherence of the washcoat was still sufficient which suggests that a 1.6% catalyst loss after the drop test (Table 5.6) is thus of sufficient adherence for use in this gas-phase test reaction.

A visual comparison of the washcoat layers after reaction as a function of lateral position (Figure 5.20) shows no noticeable variation with position and, consequently, affords no information on possible reactant flow distribution with lateral position across the microchannel reactor (Section 6.2).

5.6. Reproducibility

The reproducibility of the washcoating procedure was quantified in three ways: (1) between different channels of the same plate, (2) between different plates coated with the same suspension, and (3) between different suspensions of the same composition. A 75% Zeolite suspension was used as the reference suspension.

5.6.1. Microchannel coating reproducibility

To quantify the reproducibility of the coating in the microchannels, the thickness of the coated layer was chosen as a measurable parameter. Figure 5.21 shows the coating thickness for the first 5 microchannels on the plate. The thickness of the coatings is quantified in Figure 5.22.

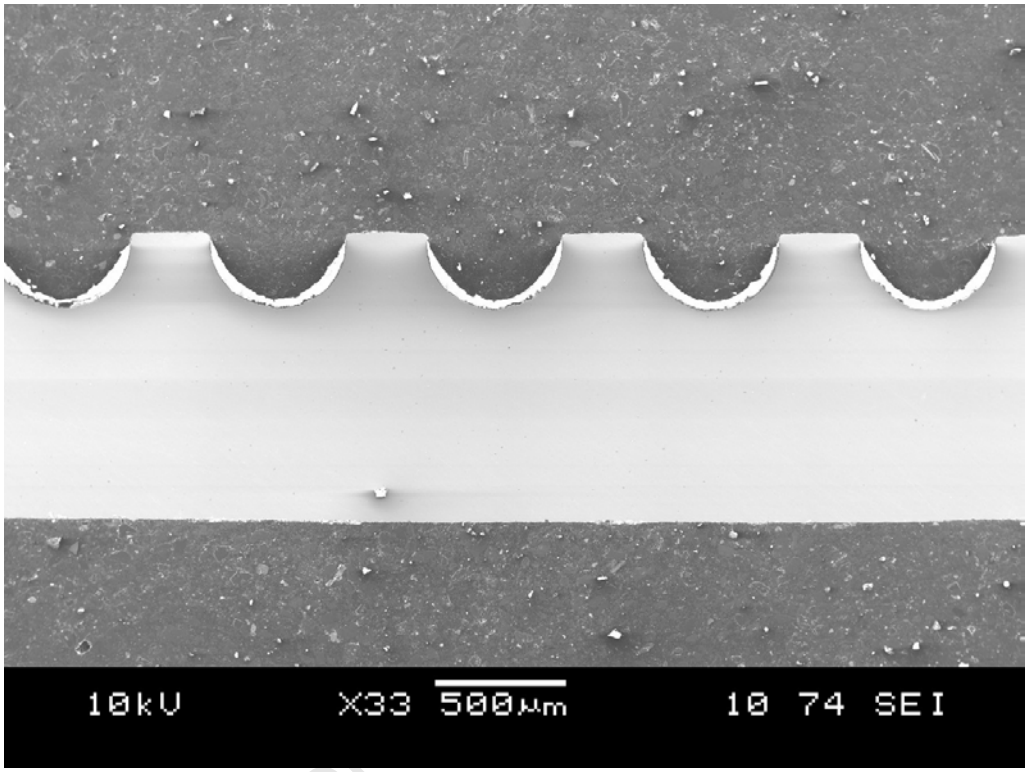

Figure 5.21: SEM image of coated microchannels with Zeolite 75 wt% washcoat.

Figure 5.22 shows the thickness of the coating on the microchannel walls and centre (bottom of the trough) of the channels, this difference in channel wall and centre thickness having been discussed in Section 5.2.3. The average wall thickness was 44 µm, whereas at the microchannel centre it was 32 µm, with average standard deviations of 4.7 µm (11 %) and 1.9 µm (6 %) respectively. The higher variability of the wall coating thickness versus that at the microchannel centre is consistent with published findings of a decrease in reproducibility with increasing catalyst loading (Mitra et al., 2008).

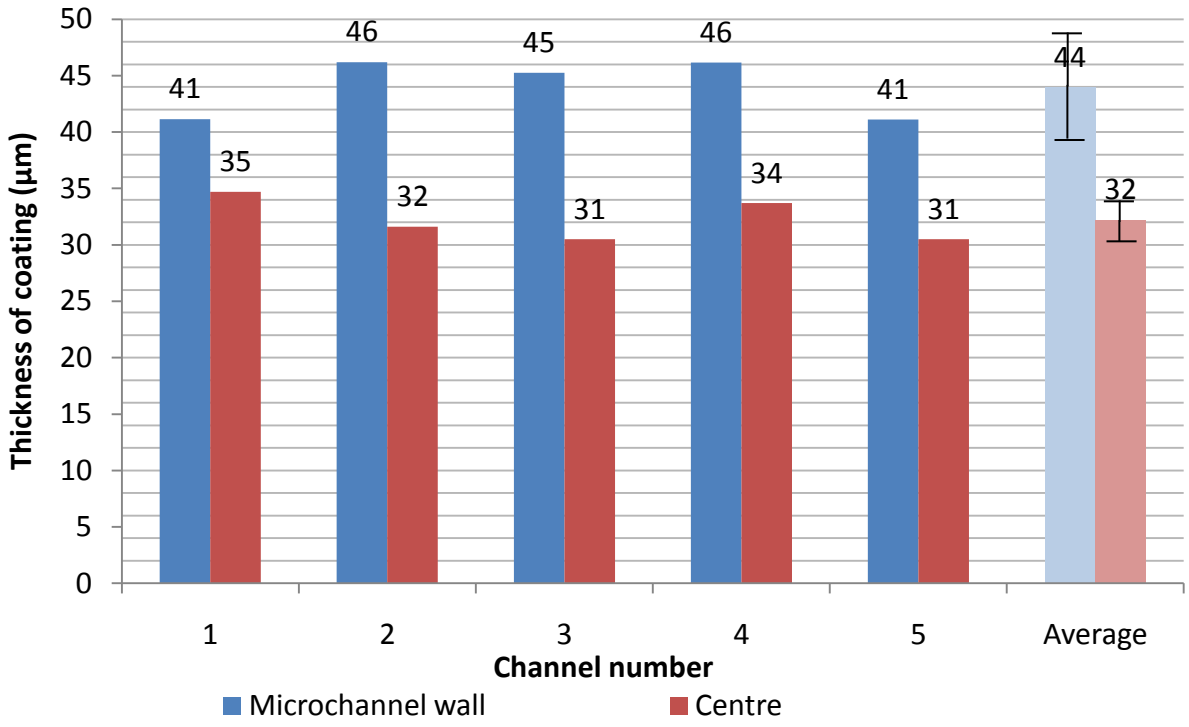

Figure 5.22: Coating thickness of the microchannels wall and centre of microchannels of a Zeolite 75% washcoat.

5.6.2. Microchannel plate reproducibility

The reproducibility of coating different microchannel plates from the same suspension was determined by measuring the coated plate weight and the amount of catalyst lost after the adherence drop test (Figure 5.23).

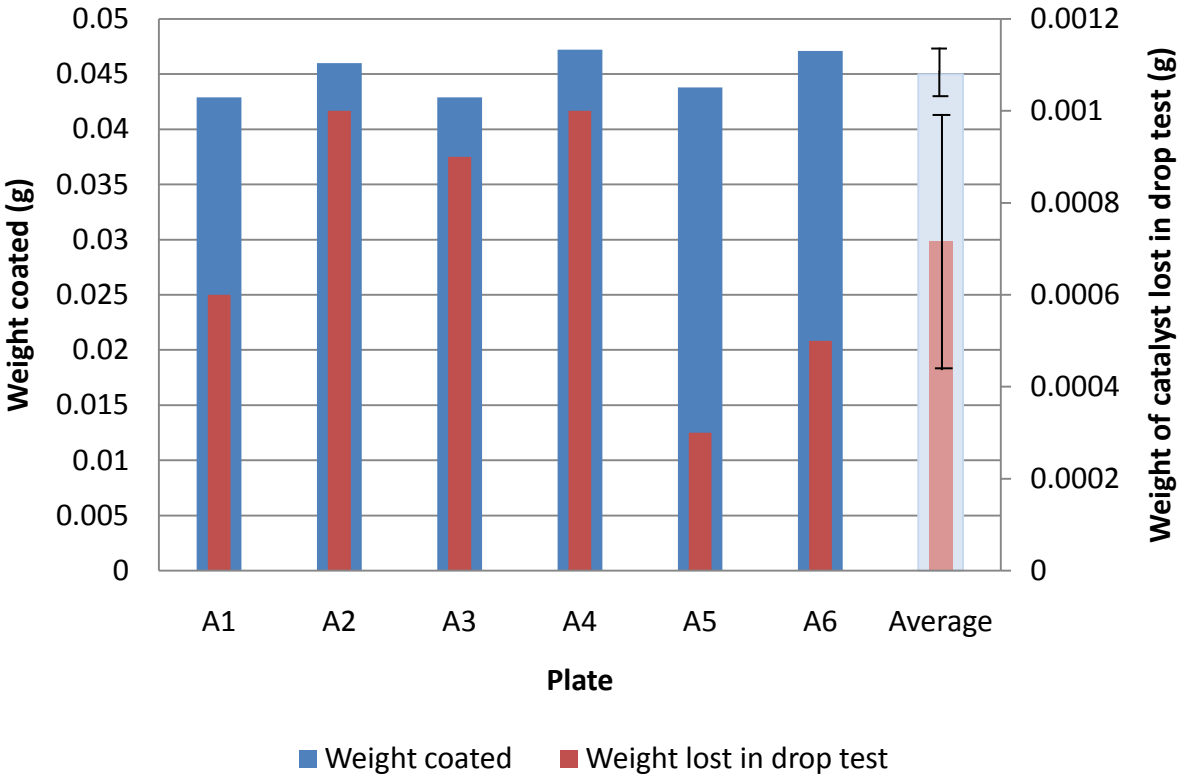

Figure 5.23: Reproducibility of coating between plates coated with Zeolite 75% washcoat.

The catalyst mass coated was 0.045 g (mean) with a standard deviation of (4 %) showing a fairly consistent washcoat mass despite a typically much greater variation in suspension viscosity (Section 5.2.3). By comparison, the average mass lost in adherence testing (0.0007 g) represents just 1.6 wt% lost, however, with a much larger variability as seen by the 43% standard deviation in this value across the six plates tested. This large variation in mass lost during the drop tests may, however, be associated with a high experimental error in recording the small amounts of weight loss on an absolute mass basis.

5.6.3. Suspension reproducibility

To quantify the suspension reproducibility, three suspensions with the same stoichiometric composition were prepared and the main suspension and coating properties compared. These suspensions used the Zeolite 75% suspension composition as a basis for comparison (Table 5.9).

Table 5.9. Reproducibility of the Zeolite 75% suspension and resulting washcoat properties.

Suspension	1	2	3	Standard Deviation	Variation (%)
[a] **Adherence test (% lost)**	1.6	1.2	1.0	0.3	24
Viscosity (cP at 50 s^{-1})	748	1005	1123	192	20
Amount coated (g)	0.0450	0.0412	0.0472	0.0030	7

[a] *Percentage mass loss of catalyst after drop tests*

Similar to the findings of Section 5.6.2, Table 5.9 indicates the amount of catalyst coated to be fairly consistent, while the drop test shows more variation between the various coated suspensions, the latter likely for the same reasons prescribed in Section 5.6.2.

The variation in suspension viscosity in Table 5.10 is large and in order to further analyse the reproducibility of the suspension viscosity, 50%, 75%, and 85% zeolite suspensions were prepared at two different times, A and B. Comparison of the suspension viscosity is given in Table 5.10.

Table 5.10: Reproducibility of suspension viscosity with varying amounts of γ-Al_2O_3 prepared at different times, A and B.

Suspension	Viscosity (cP at 50 s^{-1})	
	Time A	Time B
Zeolite 50%	614	643
Zeolite 75%	748	1005
Zeolite 85%	875	1325

Suspensions A and suspensions B were prepared at different time periods (i.e. on different days)

Each set of suspensions prepared at the same time period, either A or B, show the same trend whereby increasing the amount of γ-Al_2O_3 increases the viscosity. However, the suspensions containing the same amount of γ-Al_2O_3, but which were prepared at different times, show a rather substantial variation in suspension viscosity, this variation increasing with increasing zeolite content. The reasons for this variability with respect to preparation time is unclear and whether due to different preparation conditions such as ambient temperature, slight differences in ageing time, or stirring speed etc., it is recommended that suspensions are prepared at the same time when evaluation of properties is intended.

5.7. Influence of channel dimensions on washcoat and adherence

The impact which the channel dimensions have on the amount of catalyst coated, as well as the adhesion of the coating is illustrated in Figure 5.24. The main variant in channel dimension is the width of the channels varying from 0.3 µm to 0.75 µm. The depth of the channels is 0.25 µm for channel widths of 0.3 µm – 0.5 µm, whilst the 0.75 µm channels have a larger channel depth of 0.3 µm. (Full details of the plate dimensions are given in Section 4.2.)

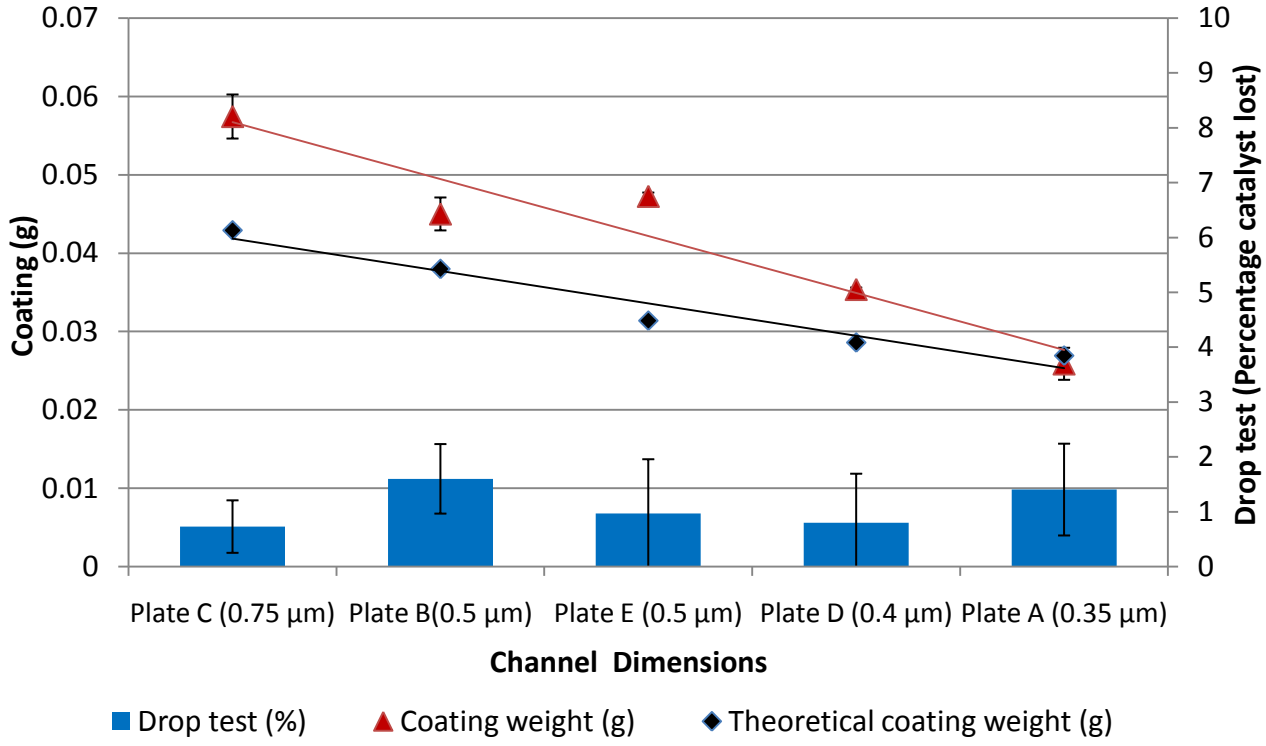

Figure 5.24: Weight of catalyst coated and adhesion on plates of varying channel width using a Zeolite 75% washcoating.

With increasing microchannel dimensions and associated increase in the amount of catalyst coated, the difference between the actual and theoretical catalyst loading increases. This difference could be attributed to a lower reproducibility with higher catalyst loading and thus greater variation from the theoretical catalyst loading (Mitra et al., 2008). The coating adhesion, however, shows no clear trend corresponding to the channel width, and thus the

data presented here shows no direct correlation with the observation in Figure 5.15 that spalling seems most prevalent at channel edges.

5.8. Other variations to coating methodology

Some variations to the Zapf et al. (2006) washcoating method were briefly evaluated with a view to improve adherence as well as to increase the zeolite loading.

5.8.1. Recoating after calcination

An additional zeolite coating was applied to the coated test plates to increase the zeolite loading. When coating the second zeolite layer, air bubbles were formed between the two zeolite coatings which could not be removed without damaging the top zeolite coating. The consequence of such air bubbles was a 'cratered' surface to the top-layer once dried and calcined as may be seen in Figure 5.25. Hence, this approach was abandoned.

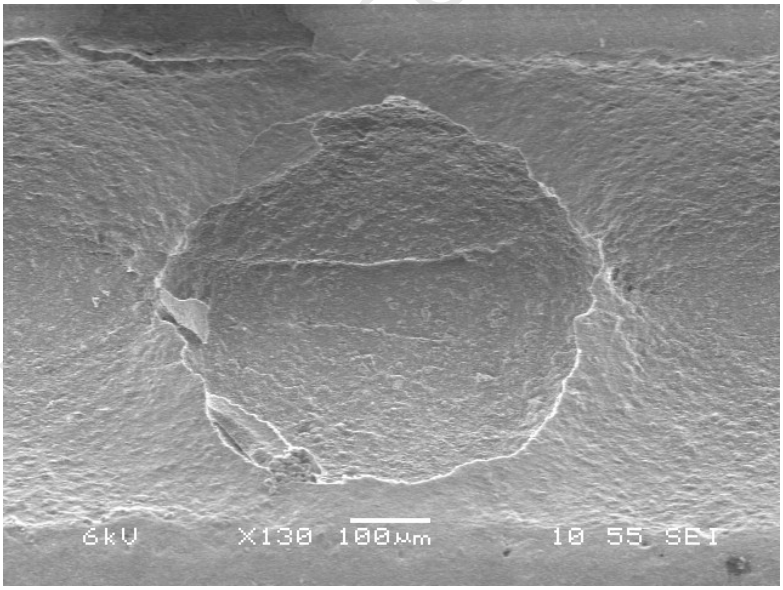

Figure 5.25: Cratering of top surface in double coating layer of directly-substituted zeolite washcoating.

5.8.2. Alumina pre-coating

Due to the γ-Al_2O_3 coating having a good adherence to the stainless steel microchannels (Section 5.2.2.2) and also a view that the zeolite coating would adhere better to a γ-Al_2O_3 pre-coat in comparison to the stainless steel surface, it was attempted to first coat the microchannels with a γ-Al_2O_3 coating followed by coating the calcined alumina layer with the directly-substituted zeolite suspension. Ultrasonification in petroleum ether resulted in the zeolite layer to peel off leaving the γ-Al_2O_3 coating behind (Figure 5.26). Consequently, the approach too was abandoned.

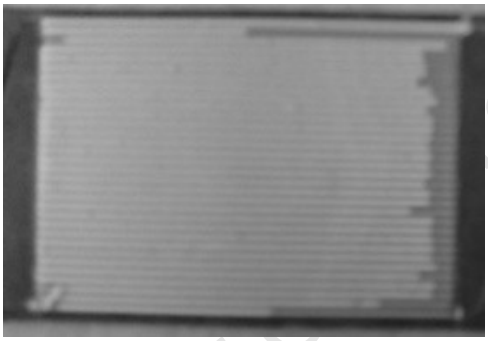

Figure 5.26: Test plate pre-coated with γ-Al_2O_3 followed by coating with directly-substituted zeolite coating after 30 minutes ultrasonification in petroleum ether.

6. Thymol synthesis

A test reaction was conducted in both the fixed-bed and microchannel reactor configurations to evaluate the performance of the respective catalysts. In the fixed-bed reactor, the performance of the simulated zeolite washcoat was compared to that of the H-MFI-90 extrudates and H-MFI-90 powder. In the microchannel reactor configuration, the washcoat performance was compared to that of the simulated washcoat in the fixed-bed configuration.

6.1. Catalyst deactivation

Deactivation of the respective catalysts was monitored by re-establishing the standard conditions so as to determine any change in catalytic performance during the interim period.

6.1.1. Catalyst stability in the fixed-bed tests

In the fixed-bed reactor configuration, the standard conditions applied were 275 ˚C, 3 bar (abs), and a feed (1:1 molar ratio of isopropanol and *m*-cresol) flow rate of 0.16 ml/min (which corresponded to different WHSV for the different catalysts). Figure 6.1 depicts the deactivation of the respective catalysts as a function of time-on-stream.

During approximately the first 100 hours of each experimental run, an initial catalyst deactivation is observed which is not unusual for hydrocarbon conversions over fresh zeolite catalysts (Ntshabele et al., 2005; Moeketsi et al., 2007; Fernsby et al., 2006; Truter and Nagooroo, 2008). After the initial deactivation, a quasi-steady state manifests. The long-term deactivation of the respective catalysts is compared in Table 6.1, where the reported values were based on the reduction in *m*-cresol conversion at the end of the experimental run.

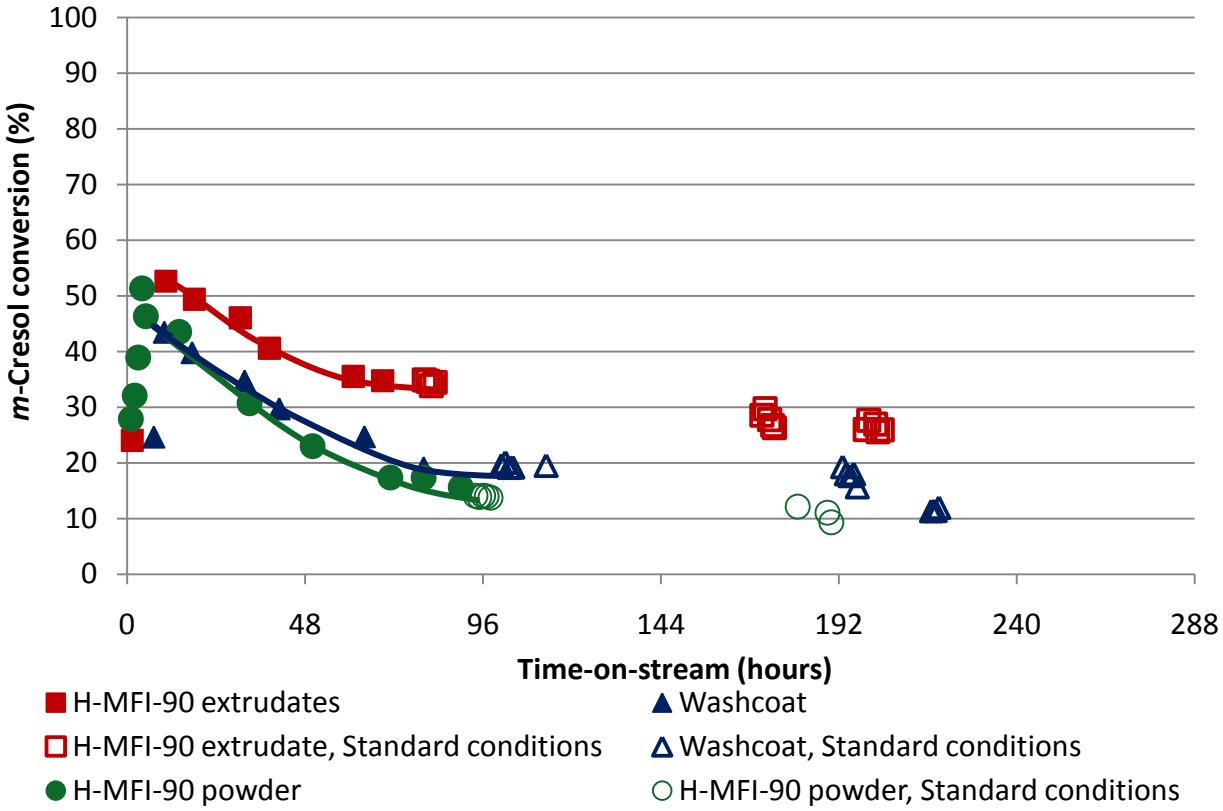

Figure 6.1: *m*-Cresol conversion vs. time-on-stream for H-MFI-90 extrudates, powder, and simulated washcoat (75 wt% Zeolite washcoat).

Table 6.1: Percentage deactivation of catalysts in fixed-bed reactor.

Catalyst	Deactivation (%)
H-MFI-90 extrudates	23
H-MFI-90 powder	33
Simulated washcoating	38

The H-MFI-90 powder and simulated washcoating deactivated by the greatest extent, whereas, the H-MFI-90 extrudates deactivated to less of an extent.

6.1.2. Catalyst stability in the microchannel tests

To evaluate the catalyst deactivation in the microchannel reactor, the WHSV was not varied since the pump was already operating close to the minimum (Appendix C). As an alternative,

the reactor temperature was varied. Figure 6.2 depicts the *m*-cresol conversion in the microchannel reactor with respect to time-on-stream and reactor temperature.

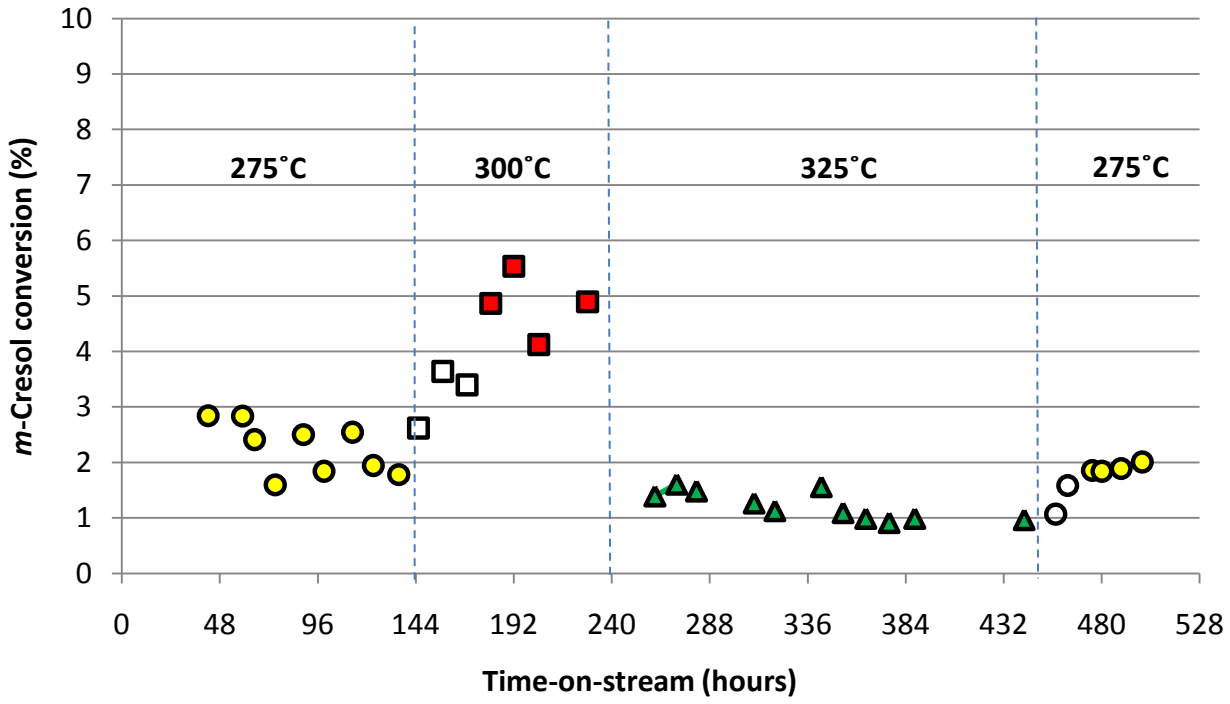

Figure 6.2: Microchannel reactor *m*-cresol conversion vs. time-on-stream with temperature variation (75 wt% Zeolite washcoat). (*Uncoloured markers indicate unsteady-state conditions.)*

The initial quasi-steady state *m*-cresol conversion at standard conditions was approximately 2%. The increase in *m*-cresol conversion with increasing temperature can be attributed to a corresponding increase in reaction rate. The decline in *m*-cresol conversion above 300 ˚C is thought to be a consequence of thermodynamic limitations due to the exothermic nature of the isopropylation reaction of *m*-cresol with isopropanol or pre-equilibrated dehydrated product (Section 2.5.5). Despite temperature variations at 300 ˚C and 325 ˚C over a period of some 300 hours, conversion returns to the initial quasi-steady state value once initial/standard conditions are re-established, indicating that catalyst performance (as measured by *m*-cresol conversion) is stable over a period of roughly 500 hours on stream and the range of conditions applied. Consequently, microchannel reactor data presented elsewhere may be considered to have been obtained under non-deactivating conditions. Futhermore, based on the limited data set of this study (Figure 6.1 and Figure 6.2), there may possibly be evidence for greater catalyst stability in the microchannel reactor configuration in comparison to the fixed-bed tests,

however, any such conclusion should be tempered by the fact that the microchannel data has been obtained at a significantly lower *m*-cresol conversion.

It should be noted that the variation in *m*-cresol conversion may mostly be attributed to the variability of feed flow rate (and, hence, space velocity) at the low pump flow rate applied (Appendix C).

6.2. Catalyst activity (*m*-Cresol conversion)

The relative activity of the respective catalysts was evaluated by comparing their *m*-cresol conversion as a function of WHSV in both the fixed-bed and microchannel reactor configurations, as shown in Figure 6.3.

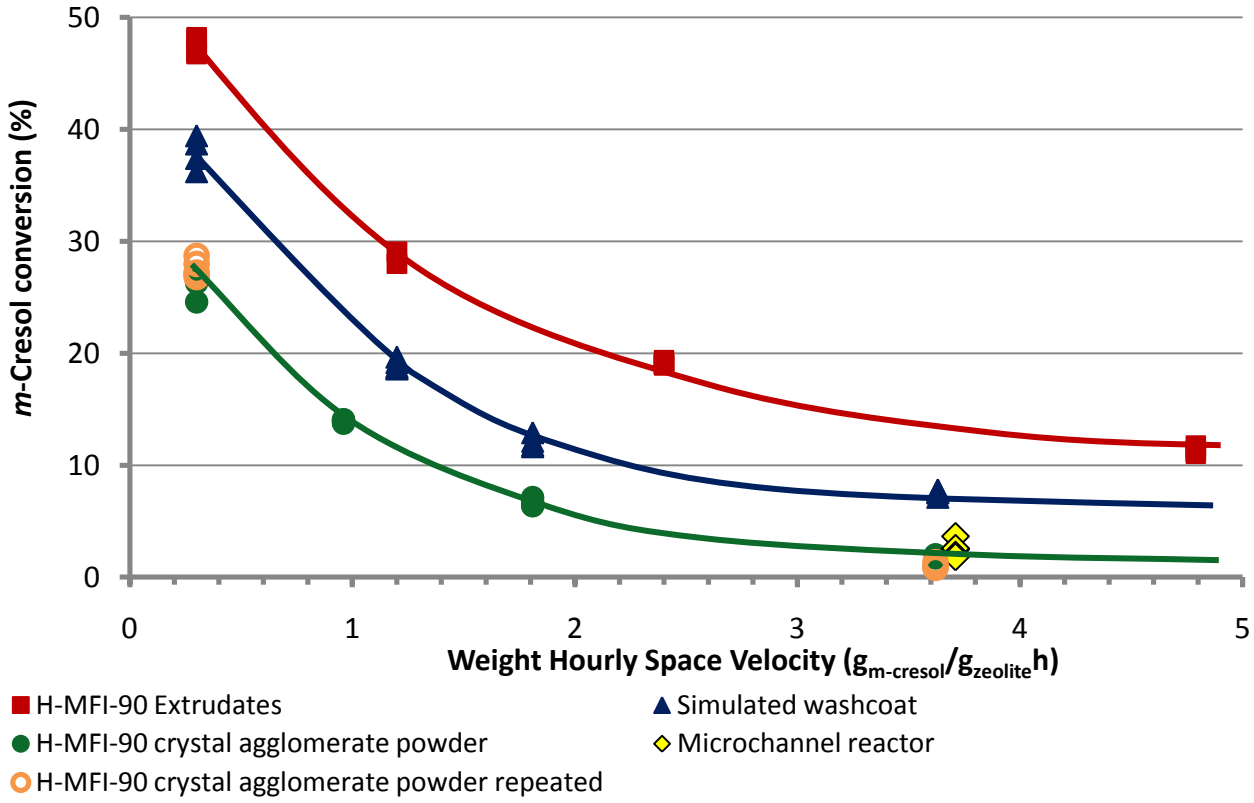

Figure 6.3: *m*-Cresol conversion vs. WHSV for H-MFI-90 extrudate, powder, simulated washcoat (fixed-bed) and the Zeolite 75% washcoat (microchannel reactor) catalysts.

The initial observation of a generally lower conversion over the powdered H-MFI-90 sample versus the H-MFI-90 extrudates was sufficiently surprising that the experiment for the H-MFI-90

powder sample was repeated at a WHSV of 0.3 $g_{m\text{-}cresol}/g_{zeolite}h$ and 3.62 $g_{m\text{-}cresol}/g_{zeolite}h$, confirming the original H-MFI-90 powder data. The H-MFI-90 extrudate data of this study is also in agreement with that of Nagooroo (2011) which confirms the validity of the H-MFI-90 extrudate data set. The difference between the H-MFI-90 extrudates and H-MFI-90 powder data series therefore appears real. The simulated washcoat data series occurs between the H-MFI-90 extrudates and powder, and despite no repeat experiment being conducted for the simulated washcoating, the four data points are consistent and show a similar trend in comparison. Therefore, assuming this data to be correct, there seems to be a notable difference between these catalysts operated in the fixed-bed configuration. To account for this difference in activity between the H-MFI-90 extrudates, H-MFI-90 powder, and simulated washcoating, several possible explanations are briefly discussed. It should, however, be noted that the explanations given are qualitative and speculative since additional experimental evidence is required to give a conclusive explanation.

Alumina binder present in both the H-MFI-90 extrudates and simulated washcoating could attribute to an additional activity. The H-MFI-90 extrudates contained a 20% γ -Al_2O_3 binder (Section 4.1), whereas the simulated washcoating contained 25% γ-Al_2O_3 binder (Section 5.2.2.2). It can be speculated that additional alumina contained in these catalysts could have resulted in the higher activity, either from the alumina binder being active in its own right due to the alumina binder containing additional acid sites and thus additional activity, or by the formation of new acid sites. It can be speculated that the formation of new acid sites could possibly have resulted from framework Si in the zeolite being substituted for Al originally contained in the binder to form new acid sites (Shihabi et al., 1985). It could be speculated that differing physical structures of the various catalysts could be considered as another possible explanation whereby different catalyst porosities influenced the catalytic activity. Fine zeolite and γ-Al_2O_3 powder used to prepare the simulated washcoat, and presumably the H-MFI-90 extrudates (exact industrial method not known), could have resulted in a different porosity of the catalyst.

In the microchannel reactor configuration, the conversion at a WHSV of 3.71 $g_{m\text{-}cresol}/g_{zeolite}h$ is lower in comparison to the simulated washcoating in the fixed-bed reactor configuration. The microchannel reactor's lower conversion cannot be attributed to catalyst deactivation as was shown in Section 6.1.1. Instead, the microchannel reactor's lower conversion may be speculated to result from poor flow distribution between the microchannels (Section 2.2.5)

causing more flow through only the middle channels and less flow in the outer channels of the microchannel reactor resulting in a lower effective residence time. However, visual inspection of the catalyst post reaction (Figure 5.18) lends no direct evidence for this possibility. As a consequence, the real reason for the apparently poorer performance in the microchannel reactor versus the fixed-bed test of the simulated coating remains unknown.

6.3. Thymol selectivity

The relative selectivity of the respective catalysts was evaluated by comparing the thymol selectivity as a function of *m*-cresol conversion in both the fixed-bed and microchannel reactor configurations, as shown in Figure 6.4.

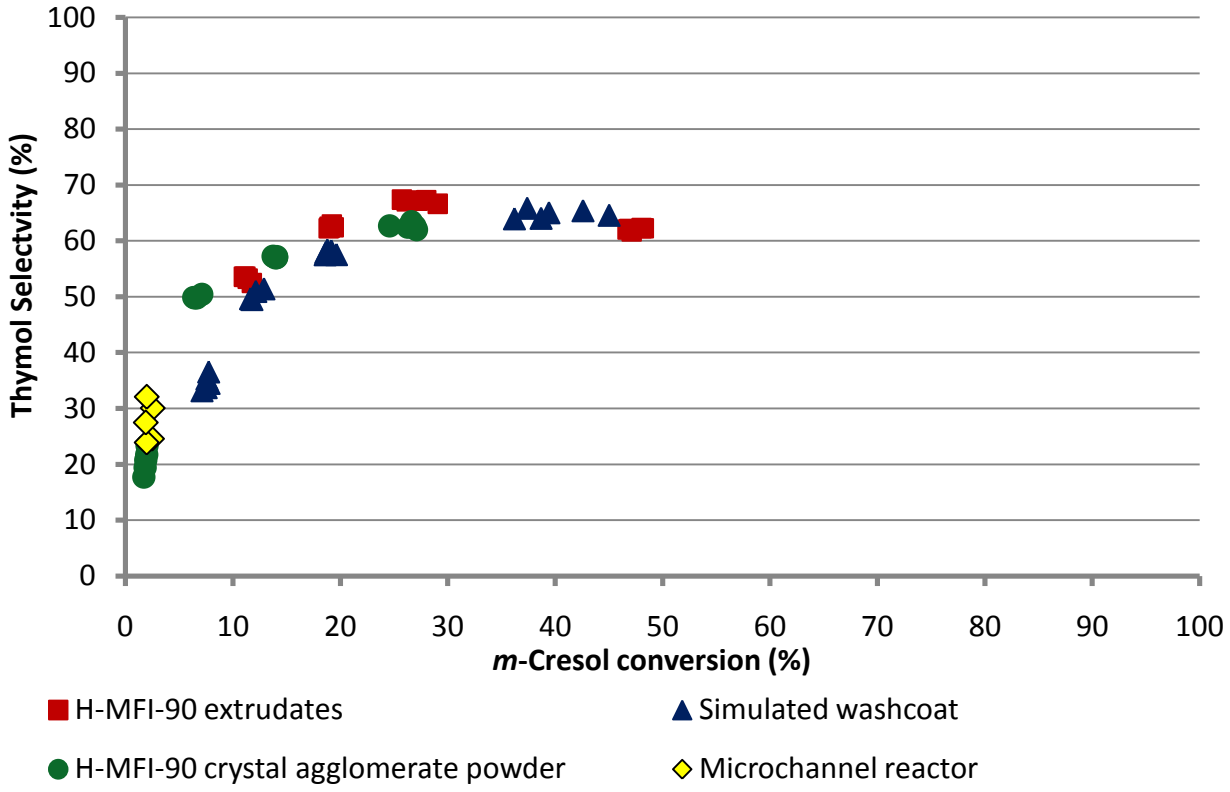

Figure 6.4: Thymol selectivity vs. *m*-cresol conversion for H-MFI-90 extrudate, powder and simulated washcoat (fixed-bed) and the Zeolite 75% washcoat (microchannel reactor) catalysts.

A comparison of the thymol selectivity data of Figure 6.4 indicates no significant variation in respect of the various catalysts, inclusive of the case for the microchannel washcoat performance, except possibly at low conversion (below 10%) where data are more subject to

error. This observation is further supported by consideration of the thymol yield data (section 6.4) for the same catalysts/tests. The findings of Shihabi et al. (1985) are similar; they too found no improvement to the original catalyst (H-MFI) selectivity despite the increase in catalytic activity caused by the addition of binder (and steaming process), albeit their observations in respect of hexane cracking.

6.4. Thymol yield

The thymol yield is presented in Figure 6.5 as a function of *m*-cresol conversion for the various catalysts and reactor configurations.

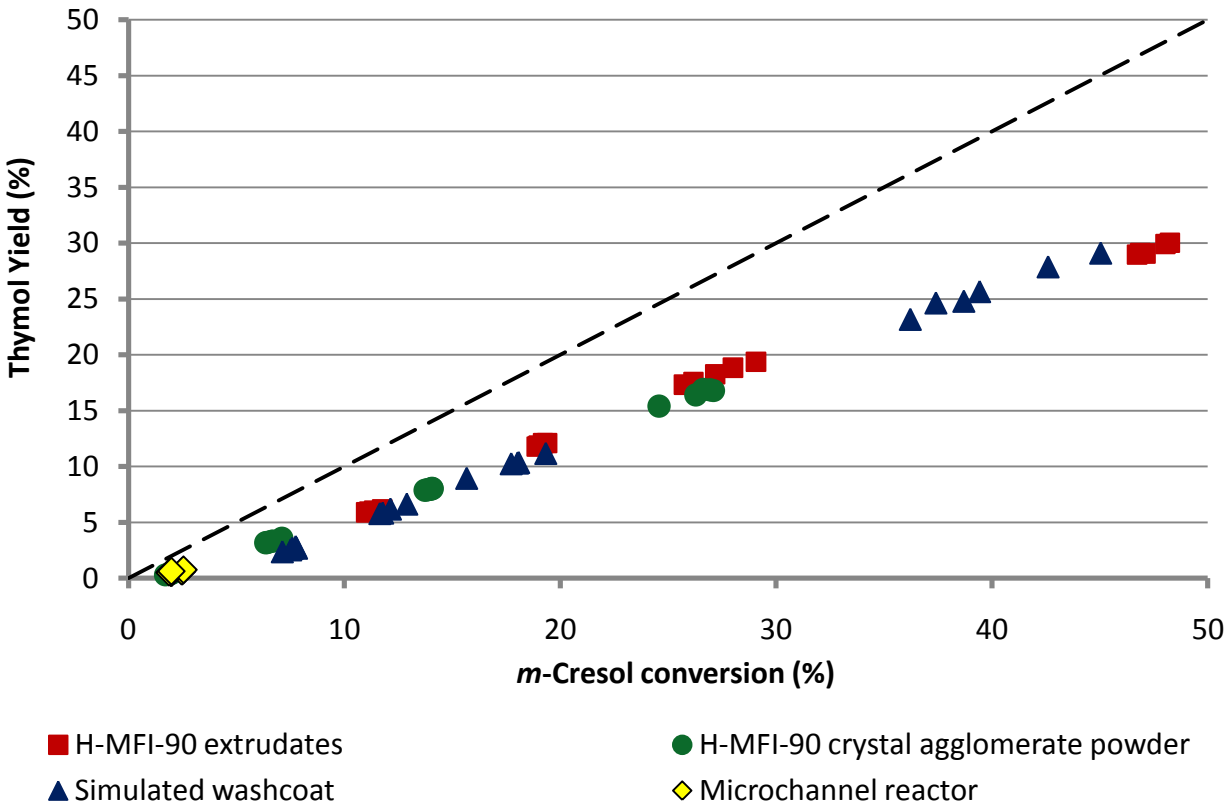

Figure 6.5: Thymol yield vs. *m*-cresol conversion for H-MFI-90 extrudate, powder and simulated washcoat (fixed-bed) and the Zeolite 75% washcoat (microchannel reactor) catalysts.

The thymol yield is found to remain constant at comparable conversions for the various catalysts in the fixed-bed configuration, and the washcoat in the microchannel reactor configuration. This is due to no change in the thymol selectivity at constant conversion (Section 6.3).

7. Conclusions

A zeolite washcoating method for stainless steel microchannel plates has been developed using the Zapf et al. (2006) washcoating technique as a basis, and applying various modifications, to obtain an adherent, active and uniform coating.

Directly substituting the zeolite crystal agglomerate powder (d_p^{ave} = 34 µm) for the γ-Al_2O_3 powder used in the Zapf et al. (2006) washcoating method resulted in a poor coating adherence with 8.1% catalyst loss after the drop test. Moreover, the zeolite suspension was found to be relatively unstable with the suspension viscosity increasing with ageing time.

One modification applied to improve the washcoat adherence was the reduction of zeolite crystal agglomerate particle size by micronising. With increasing milling time and associated smaller average particle size, a decreased suspension viscosity and increased washcoat adherence was observed. The smaller particle size permitted the formation of a tighter particle packing that, in turn, resulted in a smoother surface and better adherence after the drop test.

Another advantageous modification was the addition of a 3 µm γ-Al_2O_3 binder. An increase in γ-Al_2O_3 loading concentration improved the adherence and uniformity of the washcoat. Part of the improvement in adherence was attributed to the γ-Al_2O_3 having a lower particle size and hence reducing the average particle size of the suspension. In addition, the γ-Al_2O_3 stabilised the suspension and reduced the suspension viscosity which, consequently, improved coating uniformity. The possibility of the washcoat adherence being dependant on the suspension viscosity was considered due to a reduction in viscosity showing a corresponding improvement in adherence. Lowering the suspension viscosity was thought to aid in the improvement of the washcoat uniformity and thus decreased the amount of spalling from the washcoat, specifically on the microchannel walls. The addition of 25% γ-Al_2O_3 was found to be the best compromise

between improving the coating adherence and suspension stability, and minimizing the loss of the overall coating activity, BET surface area and crystallinity.

The incorporation of both the reduction of zeolite powder particle size, as well as the addition of γ-Al_2O_3 binder aided in the maximum zeolite washcoat adherence, with only 0.1% catalyst mass loss after the drop test. However, evaluation of a Zeolite 75% washcoat, without reduced particle size, after the thymol synthesis reaction, showed no visible catalyst loss implying that for this specific reaction no zeolite milling is required and a catalyst loss of only 1.6% after the drop test is adequate.

As an additional adherence test to evaluate the coating adherence in the presence of a liquid, the coated microchannel plates were subjected to an ultrasonification test in petroleum ether and isopropanol. In general, the ultrasonification tests indicated a greater percentage catalyst mass loss when compared to the drop test, however, the same trend of increasing γ-Al_2O_3 corresponding to an improvement in the coating adherence could be observed.

A statistical study of the washcoating method found the amount of catalyst coated (approximately 45 mg) to have a good reproducibility with an average variation of only 4% between plates. The washcoat thickness varied between 30 μm and 46 μm with the microchannel walls being thicker; potentially because of the higher suspension viscosity. The reproducibility of the coating thickness was found to be satisfactory with the microchannel walls having a lower reproducibility due to the higher catalyst loading. Coating adherence and suspension viscosity were the least reproducible coating properties. The variation in washcoat adhesion between different plates was thought to be attributed to the high experimental error associated with recording the small amount of weight loss and total catalyst loading. The variation in the suspension viscosity was thought to be caused as a result of different preparation conditions. It is recommended that the suspensions be prepared simultaneously when trends between different suspensions are to be compared.

Evaluation of the zeolite crystal structure and size by X-ray diffraction of the original zeolite crystal agglomerate powder, directly-substituted zeolite washcoat, and milled zeolite washcoat showed no significant difference, indicating that the essential zeolite catalyst is not affected to any significant extent as a consequence of the washcoat preparation.

To further assess whether the zeolite washcoat underwent any changes in catalytic activity, a test reaction was conducted. Evaluation of a simulated washcoating in the fixed-bed reaction in comparison to the original H-MFI-90 powder indicated that the washcoating method did not cause any detrimental affects to the zeolite activity, in fact, an improvement in washcoat activity was observed over the original catalysts on a per mass zeolite basis. A possible explanation for this improvement was attributed to the presence of the γ-Al_2O_3 binder in the simulated washcoating or changes in porosity of the various catalysts.

No improvements in thymol yield were observed in the microreactor when compared to the fixed-bed reactor. The thymol selectivity and yield of the respective catalysts and reactor configurations were found to be relatively comparable with respect to *m*-cresol conversion. It may be speculated that the possibility of poor flow distribution may potentially be a partial explanation for the observed findings. It is recommended that further use of the zeolite washcoating technique in microchannels reactors be applied to high reaction rate reactions in order to fully utilize the benefits obtainable in the microchannel reactor.

8. References

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Appendix

A.

A.1 Adherence and coating data

Data of the test plates before coating, after coating, and after the adherence tests are given in this section for the various suspensions.

Table A.1: Data of plate weights before and after drop test and percentage catalyst lost in drop test.

	Uncoated plate (g)	Coated plate (g)	Coated plate after drop test (g)	Catalyst coated (g)	Catalyst lost drop test (g)	Percentage catalyst lost drop test (%)
Zeolite -A (10.7 um)	*12.5702*	*12.6133*	*12.6127*	0.0431	0.0006	1.39
	12.7064	*12.7497*	*12.7482*	0.0433	0.0015	3.46
Zeolite -B (7.2 um)	*12.5707*	*12.6065*	*12.6063*	0.0358	0.0002	0.56
	12.7097	*12.7414*	*12.7411*	0.0317	0.0003	0.95
	12.7223	*12.7521*	*12.7515*	0.0298	0.0006	2.01
	12.5763	*12.6129*	*12.6123*	0.0366	0.0006	1.64
Zeolite -C (9.56 um)	*12.6218*	*12.6616*	*12.6601*	0.0398	0.0015	3.77
	12.5594	*12.6077*	*12.6072*	0.0483	0.0005	1.04
	12.6087	*12.6516*	*12.6510*	0.0429	0.0006	1.40
	12.6017	*12.6470*	*12.6458*	0.0453	0.0012	2.65
Silica C	*12.6034*	*12.6546*	*12.6401*	0.0512	0.0329	64.26
	12.4803	*12.5287*	*12.5154*	0.0484	0.0343	70.87
	12.6026	*12.6523*	*12.6407*	0.0497	0.0328	66.00
	12.6047	*12.6520*	*12.6471*	0.0473	0.0290	61.31
	12.5783	*12.6266*	*12.6220*	0.0483	0.0260	53.83
Zeolite 75% - A	*12.6685*	*12.7159*	*12.7158*	0.0474	0.0001	0.21
	12.5458	*12.5927*	*12.5927*	0.0469	0.0000	0.00
	12.5712	*12.6201*	*12.6199*	0.0489	0.0002	0.41
	12.5307	*12.5809*	*12.5809*	0.0502	0.0000	0.00
Zeolite 75% - B	*12.4775*	*12.5259*	*12.5258*	0.0484	0.0001	0.22
	12.6230	*12.6674*	*12.6673*	0.0444	0.0001	0.23
	12.4356	*12.4853*	*12.4853*	0.0497	0.0000	0.00
	12.6305	*12.6978*	*12.6977*	0.0673	0.0001	0.15

Table A.2: Data of plate weights before and after drop test and ultrasonification tests for suspensions containing alumina binder.

	Plate uncoated (g)	Coated plate (g)	Plate after drop test (g)	Plate after Petroleum Ether	Plate after Isopropanol	Catalyst coated (g)	Catalyst lost drop test (g)	Catalyst lost Petrolem ether (g)	Catalyst lost Isopropanol (g)
Directly-substituted (Zeolite 100%)	*12.5660*	*12.6088*	*12.6085*	*12.5854*	*12.5820*	0.0428	0.0003	0.0234	0.0268
	12.6275	*12.6706*	*12.6639*	*12.6295*	*12.6280*	0.0431	0.0067	0.0411	0.0426
	12.4432	*12.4885*	*12.4845*	*12.4573*	*12.4523*	0.0453	0.0040	0.0312	0.0362
	12.5677	*12.6088*	*12.6072*	*12.5732*	*12.5691*	0.0411	0.0016	0.0356	0.0397
	12.6473	*12.6896*	*12.6839*	*12.6497*	*12.6488*	0.0423	0.0057	0.0399	0.0408
Zeolite 90%	*12.6074*	*12.6528*	*12.6498*	*12.6466*	*12.6307*	0.0454	0.0030	0.0062	0.0221
	12.6296	*12.6756*	*12.6716*	*12.6564*	*12.6518*	0.0460	0.0040	0.0192	0.0238
	12.6223	*12.6611*	*12.6610*	*12.6598*	*12.6578*	0.0388	0.0001	0.0013	0.0033
	12.6249	*12.6664*	*12.6659*	*12.6652*	*12.6361*	0.0415	0.0005	0.0012	0.0303
	12.5931	*12.6341*	*12.6339*	*12.6323*	*12.6311*	0.0410	0.0002	0.0018	0.0030
Zeolite 85%	*12.5703*	*12.6169*	*12.6161*	*12.6152*	*12.6121*	0.0466	0.0008	0.0017	0.0048
	12.6309	*12.6729*	*12.6723*	*12.6710*	*12.6690*	0.0420	0.0006	0.0019	0.0039
	12.6039	*12.6458*	*12.6455*	*12.6454*	*12.6410*	0.0419	0.0003	0.0004	0.0048
	12.6234	*12.6634*	*12.6630*	*12.6632*	*12.6532*	0.0400	0.0004	0.0002	0.0102
	12.6274	*12.6698*	*12.6674*	*12.6668*	*12.6651*	0.0424	0.0024	0.0030	0.0047
Zeolite 75%	*12.6087*	*12.6516*	*12.6510*	*12.6512*	*12.6506*	0.0429	0.0006	0.0004	0.0010
	12.7105	*12.7565*	*12.7555*	*12.7543*	*12.7522*	0.0460	0.0010	0.0022	0.0043
	12.5773	*12.6202*	*12.6193*	*12.6194*	*12.6156*	0.0429	0.0009	0.0008	0.0046
	12.6249	*12.6721*	*12.6711*	*12.6660*	*12.6660*	0.0472	0.0010	0.0061	0.0061
	12.6224	*12.6662*	*12.6659*	*12.6661*	*12.6648*	0.0438	0.0003	0.0001	0.0014
	12.4953	*12.5424*	*12.5419*	*12.5431*	*12.5410*	0.0471	0.0005	0.0007	0.0014
Zeolite 50%	*12.5594*	*12.6077*	*12.6072*	*12.6061*	*12.6054*	0.0428	0.0005	0.0016	0.0023
	12.5761	*12.6208*	*12.6207*	*12.6199*	*12.6195*	0.0431	0.0001	0.0009	0.0013
	12.6017	*12.6470*	*12.6458*	*12.6460*	*12.6465*	0.0453	0.0012	0.0010	0.0005
	12.7244	*12.7661*	*12.7658*	*12.7624*	*12.7581*	0.0411	0.0003	0.0037	0.0080
	12.6364	*12.6788*	*12.6785*	*12.6774*	*12.6749*	0.0423	0.0003	0.0014	0.0039
	12.6028	*12.6430*	*12.6429*	*12.6428*	*12.6426*	0.0454	0.0001	0.0002	0.0004
Alumina	*12.6257*	*12.6692*	*12.6688*	*12.6677*	*12.6661*	0.0460	0.0004	0.0015	0.0031
	12.5004	*12.6077*	*12.6076*	*12.6076*	*12.6056*	0.0388	0.0001	0.0001	0.0021
	12.6131	*12.6566*	*12.6566*	*12.6563*	*12.6557*	0.0415	0.0000	0.0003	0.0009
	12.5724	*12.6171*	*12.6170*	*12.6163*	*12.6157*	0.0410	0.0001	0.0008	0.0014
	12.5522	*12.6248*	*12.6244*	*12.6232*	*12.6230*	0.0466	0.0004	0.0016	0.0018
	12.5061	*12.5469*	*12.5468*	*12.5463*	*12.5448*	0.0420	0.0001	0.0002	0.0021

Table A.3: Percentage of catalyst lost for the drop test and ultrasonification tests for suspensions containing alumina binder.

Suspension	Catalyst lost drop test (%)	Catalyst lost Petroleum ether (%)	Catalyst lost Isopropanol (%)
Directly-substituted (Zeolite 100%)	0.70	54.67	62.62
	15.55	95.36	98.84
	8.83	68.87	79.91
	3.89	86.62	96.59
	13.48	94.33	96.45
Zeolite 90%	6.61	13.66	48.68
	8.70	41.74	51.74
	0.26	3.35	8.51
	1.20	2.89	73.01
	0.49	4.39	7.32
Zeolite 85%	1.72	3.65	10.30
	1.43	4.52	9.29
	0.72	0.95	11.46
	1.00	0.50	25.50
	5.66	7.08	11.08
Zeolite 75%	1.40	0.93	2.33
	2.17	4.78	9.35
	2.10	1.86	10.72
	2.12	12.92	12.92
	0.68	0.23	3.20
	1.06	1.49	2.97
Zeolite 50%	1.04	3.31	4.76
	0.22	2.01	2.91
	2.65	2.21	1.10
	0.72	8.87	19.18
	0.71	3.30	9.20
	0.25	0.50	1.00
Alumina	0.92	3.45	7.13
	0.09	0.09	1.96
	0.00	0.69	2.07
	0.22	1.79	3.13
	0.55	2.20	2.48
	0.25	0.49	5.15

Table A.4: Average amount of catalyst coated and catalyst lost after various adherence tests for all suspensions.

	Catalyst coated (g)	Percentage catalyst lost drop test (wt%)	Catalyst lost after petroleum ether ultrasonification (wt%)	Catalyst lost after isopropanol ultrasonification (wt%)
Zeolite -A (10.7 um)	0.0432	2.4	-	-
Zeolite -B (7.2 um)	0.0335	1.3	-	-
Zeolite C- (9.56 um)	0.0455	2.2	-	-
Silica -C	0.0490	63	-	-
Zeolite 75% - A	0.0472	0.2	-	-
Zeolite 75% - B	0.0464	0.1	-	-
Zeolite 100%	0.0430	8.1	66.9	80.7
Zeolite 90%	0.0429	3.5	14.0	45.8
Zeolite 85%	0.0426	2.1	1.0	11.3
Zeolite 75%	0.0450	1.6	2.1	6.9
Zeolite 50%	0.0438	0.9	2.4	6.4
Alumina	0.0587	0.3	1.0	2.5

Table A.5: Data of plate weights before and after drop test and percentage lost in drop test for plates of different dimensions.

	Plate uncoated (g)	Coated plate (g)	Plate after drop test (g)	Catalyst coated (g)	Drop test (g)	Drop test (%)
Plate A	*12.4745*	*12.5200*	*12.5190*	0.0455	0.0010	2.20
	12.6660	*12.7163*	*12.7161*	0.0503	0.0002	0.40
	12.4326	*12.4793*	*12.4792*	0.0467	0.0001	0.21
	12.4878	*12.5343*	*12.5337*	0.0465	0.0006	1.29
	12.6064	*12.6502*	*12.6457*	0.0438	0.0045	10.27
Plate D	*12.9107*	*12.9454*	*12.9450*	0.0347	0.0004	1.15
	12.8837	*12.9177*	*12.9172*	0.0340	0.0005	1.47
	12.8645	*12.9040*	*12.9039*	0.0395	0.0001	0.25
	12.9800	*13.0121*	*13.0117*	0.0321	0.0004	1.25
	12.9184	*12.9550*	*12.9548*	0.0366	0.0002	0.55
Plate E	*13.3790*	*13.4042*	*13.4037*	0.0252	0.0005	1.98
	13.3086	*13.3330*	*13.3327*	0.0244	0.0003	1.23
	13.2801	*13.3071*	*13.3067*	0.027	0.0004	1.48
	13.3252	*13.3510*	*13.3504*	0.0258	0.0006	2.33
	13.2622	*13.2891*	*13.2891*	0.0269	0.0000	0.00
Plate C	*11.9150*	*11.9739*	*11.9737*	0.0589	0.0002	0.34
	11.8291	*11.8867*	*11.8853*	0.0576	0.0014	2.43
	11.8326	*11.8884*	*11.8880*	0.0558	0.0004	0.72
	11.0210	*11.0810*	*11.0806*	0.0600	0.0004	0.67
	11.0169	*11.0755*	*11.0748*	0.0586	0.0007	1.19

Table A.6: Summary of coating weight for plates of different dimensions.

	Coating	Drop test (wt%)	Theoretical Coating weight
Plates C (0.75µm)	0.0574	1.07	0.0429
Plates E (0.5 µm)	0.0403	1.02	0.0314
Plates D (0.4 µm)	0.0354	0.93	0.0286
Plates A (0.35 µm)	0.0259	1.40	0.0269

A.2 Calculation of theoretical coating weight

This section gives the calculations necessary to determine the theoretical amount of catalyst coated per test plate.

Channel dimensions:

Channel depth: 0.3 mm
Channel width: 0.5 mm
Length of channels: 50 mm
Number of channels: 32

As an example plate B, is used to explain the method of calculation. Due to the difference in channel height and depth; an upper, lower and average loading was calculated. The volume of the microchannel test plate is calculated to be 0.1788 cm^3 (average limit). Using the density of the zeolite (1.063 g/cm^3) the weight of the suspension per plate could be calculated. With a 20% solids concentration in the suspension, the theoretical amount of catalyst per plate is 0.0380 g. Similar calculations for the other plate dimensions are summarized in the table below.

Table A.7: Theoretical weight of catalyst per test plate.

Plate name	Plate B: lower limit	Plate B: average limit	Plate B: upper limit
Channel Width (mm)	0.5	0.5	-
Channel Depth (mm)	-	0.3	0.3
Channel area (mm^3)	4.9087	5.9396	7.0686
Plate area (mm^3)	157.08	190.07	226.19
Plate area (cm^3)	0.1478	0.1788	0.2128
Plate coating (g)	0.1570	0.1900	0.2261
20% solids concentration coating (g)	0.0314	0.0380	0.0452

A.3 Calculation of microchannel plate surface area

The microchannel plate surface area was calculated using the general equation stated below.

$$\text{Plate surface area} = \pi \times (\text{Channel radius}) \times (\text{Length of Channels}) \times (\text{Number of channels})$$

Equation A.1: Calculation of test plate surface area.

For plate B, the radius varied between channel depth of 0.3 mm and half of the channel width being 0.5 mm. The upper and lower limits were therefore between 12.5 cm^2 and 15.1 cm^2.

Appendix

B.

B.1 Microchannel reactor plates

The 75% zeolite washcoating (microchannel reactor plates B and C) were evaluated in the microchannel reactor. In addition to these microchannel reactors, various other microchannel reactors with other washcoating compositions were made. The details of these plates are given below.

Table B.1: Summary of microchannel reactors produced.

Microchannel reactor	Total coating [a](g)	H-MFI-90 zeolite (wt%)	Zeolite average particle size (μm)	γ-Al_2O_3 (wt %)
A	0.0251	75[a]	8	25
B*	0.0256	75	34	25
C*	0.0251	75	34	25
D	0.0247	75	34	25
E	0.0257	50	34	50
F	0.0264	50	34	50
G	0.0241	90	34	10
H	0.0241	90	34	10
I	0.0248	90	34	10

[a] The theoretical microreactor loading is 0.0285 g.

* These microreactors were used in this study.

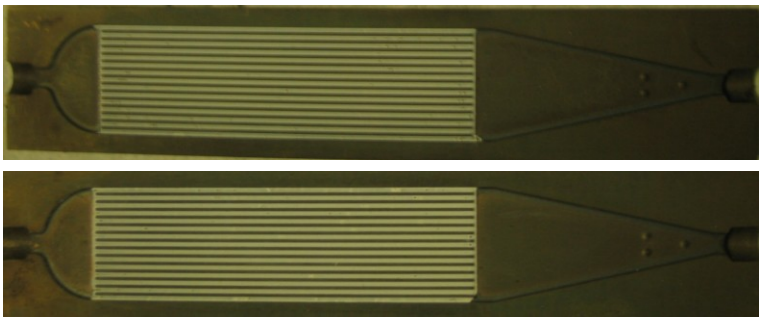

Figure B.1: Microchannel reactor plates: A. Composition: 75 wt% H-MFI-90 (8 µm) reduced zeolite particle size powder and 25 wt% γ-Al_2O_3.

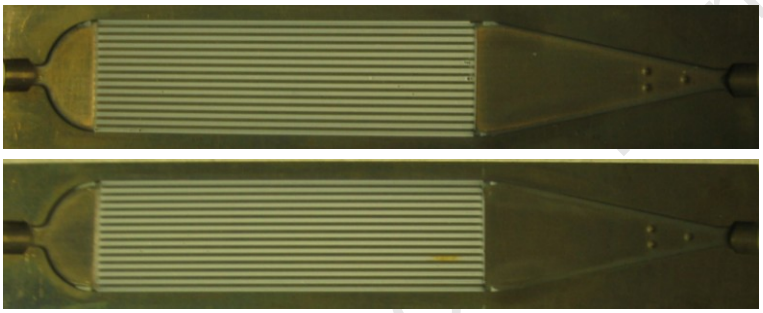

Figure B.2: Microchannel reactor plates: B. Composition: 75 wt% H-MFI-90 powder and 25 wt% γ-Al_2O_3 (Used in study).

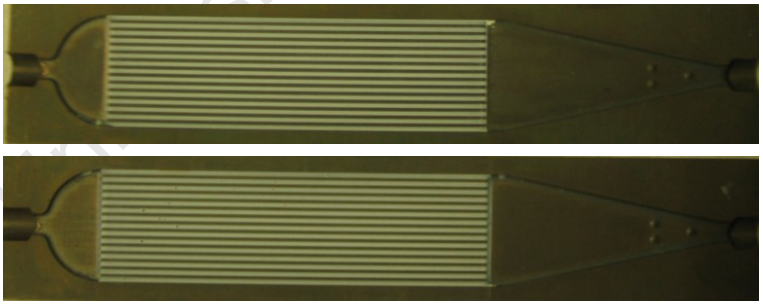

Figure B.3: Microchannel reactor plates: C. Composition: 75 wt% H-MFI-90 powder and 25 wt% γ-Al_2O_3 (Used in study).

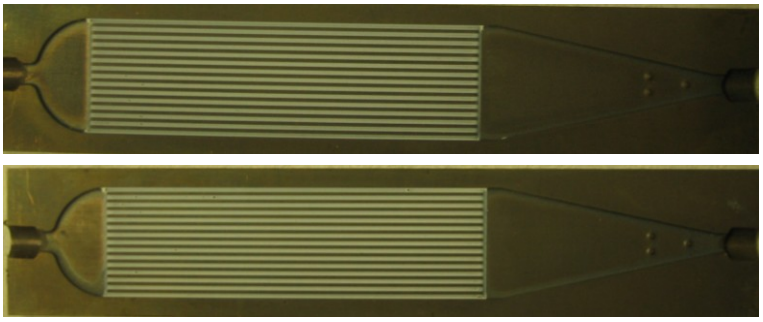

Figure B.4: Microchannel reactor plates: D. Composition: 75 wt% H-MFI-90 powder and 25 wt% γ-Al_2O_3.

Figure B.5: Microchannel reactor plate: E1. Composition: 50 wt% H-MFI-90 powder and 50 wt% γ-Al_2O_3 (Microchannel reactor plate E2 image not included due to poor photo quality image).

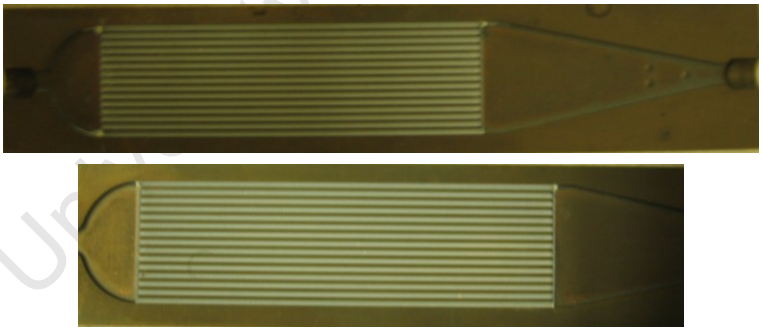

Figure B.6: Microchannel reactor plates: F. Composition: 50 wt% H-MFI-90 powder and 50 wt% γ-Al_2O_3.

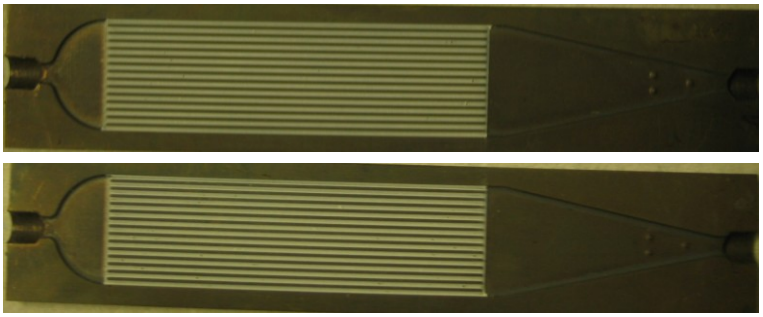

Figure B.7: Microchannel reactor plates: G. Composition: 90% H-MFI-90 powder and 10% γ-Al_2O_3.

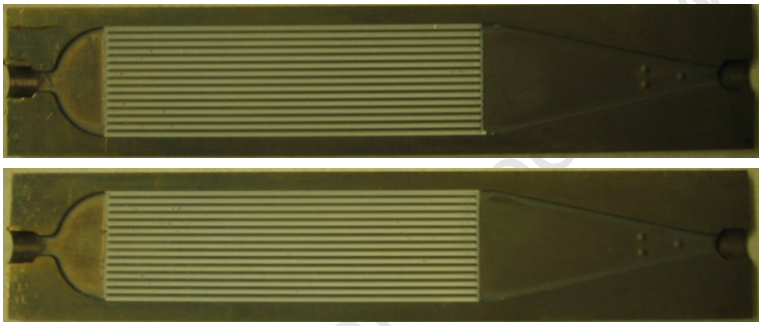

Figure B.8: Microchannel reactor plates: H. Composition: 90 wt% H-MFI-90 powder and 10 wt% γ-Al_2O_3.

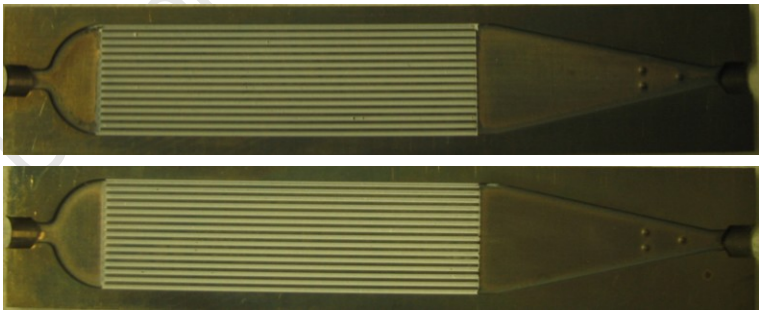

Figure B.9: Microchannel reactor plates: I. Composition: 90 wt% H-MFI-90 powder and 10 wt% γ-Al_2O_3.

Appendix

C.

C.1 Relevance of valve V- 4

The importance of valve V-4 should be noted. Initially, this valve was not incorporated into the rig design which resulted in large fluctuations in conversion due to the reagents vapourising (essentially the isopropanol) in the reactor head (Figure 4.16). Due to there being a temperature gradient between the reactor head and guard catch pot GCP-1 (at ambient temperature), the vapourous isopropanol diffused from the reactor head through the nitrogen line to the cooler guard catch pot and condensed. This was particularly evident during the evenings when a larger temperature gradient existed resulting in a more pronounced depletion of the feed mixture of isopropanol and, hence, lower conversion of *m*-cresol.

C.2 Pump functionality at low flow rates

Operating the pump at low flow rates, close to the pump minimum of 0.001 ml/min, resulted in large fluctuations. A comparison of the fluctuations in flow rate is shown for a 0.002 ml/min (Figure C.1 and a 0. 002 ml/min (Figure C.2).

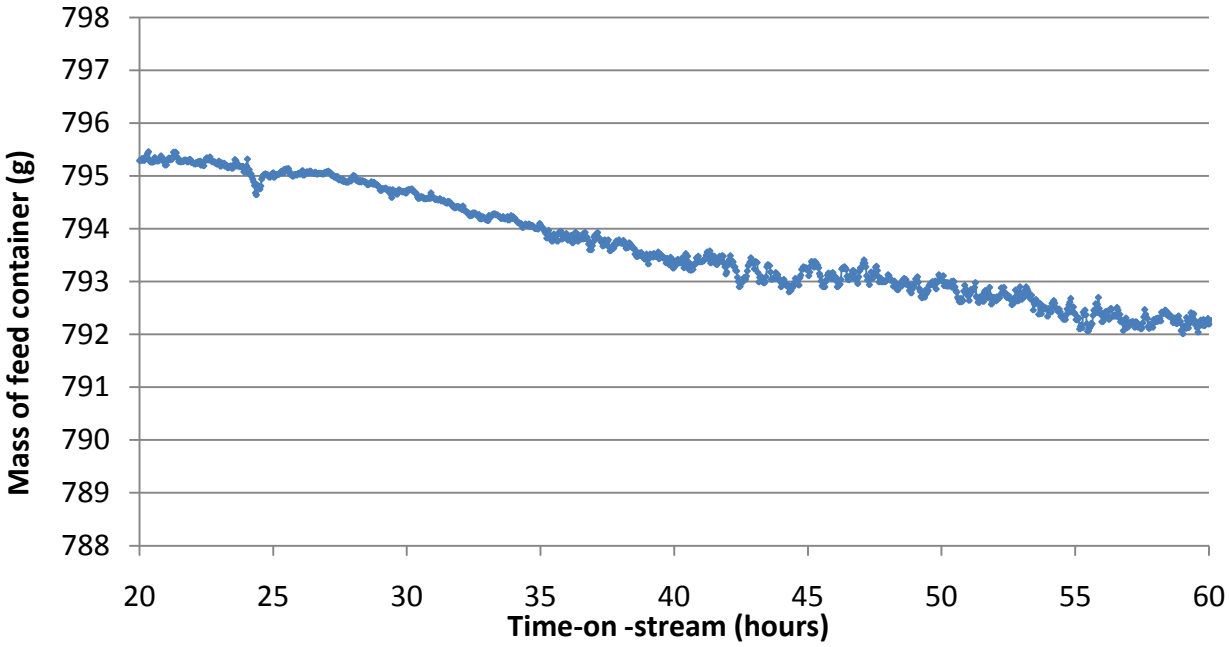

Figure C.1: Mass of feed container with respect to time-on-stream in the microchannel reactor configuration at pump flow rate of 0.002 ml/min.

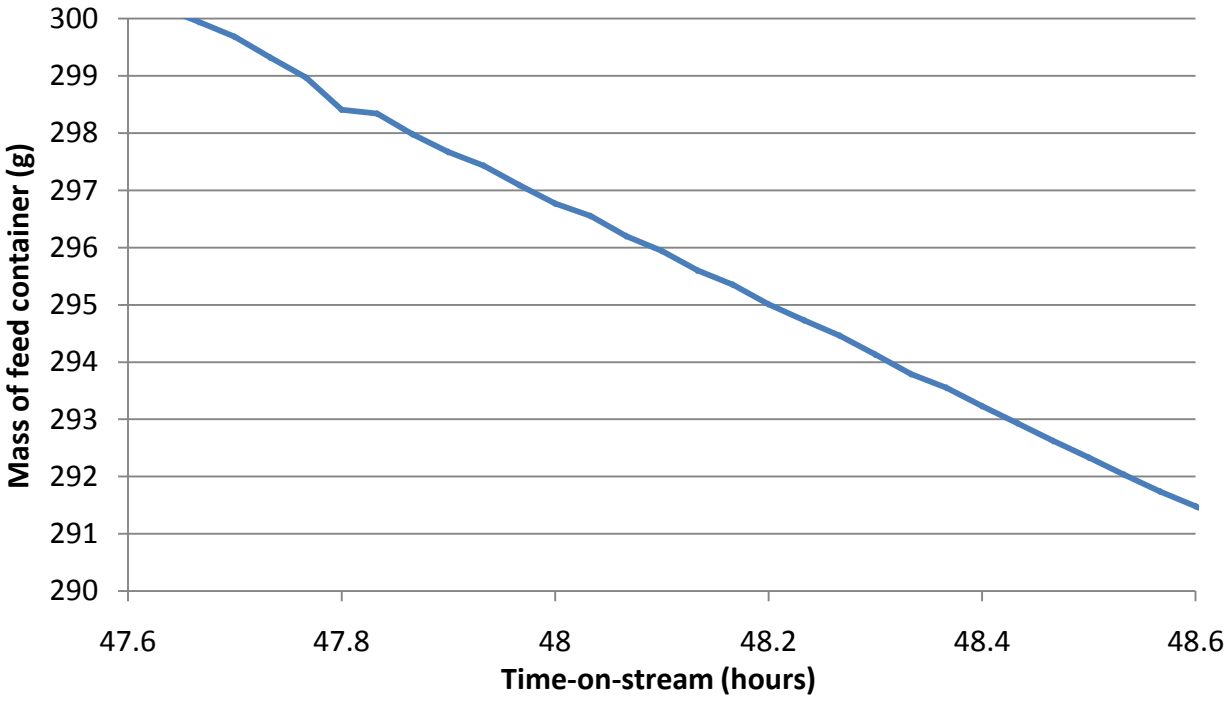

Figure C.2: 10 g mass loss of feed container with respect to time-on-stream in the fixed-bed configuration at a pump flow rate of 0.16 ml/min.

The mass of the feed container was recorded with respect to time-on-stream to evaluate the extent of these flow rate fluctuations. At a low flow rate of 0.002 ml/min, there is a large variation in the feed flow rate in comparison to higher flow rates of 0.16 ml/min. More variation in sample compositions were therefore seen in the microchannel reactor configuration.

C.3 Microsplitter

A microsplitter was used in order to reduce the flow rate below the pump minimum. However, at a flow rate below 0.001 ml/min, no product sample was recovered. It was thought that the volume of the fluid lines between the pump and the microchannel reactor, and the microchannel reactor and product catch pot were too large for this small flow rate. The feed and product therefore accumulated in these lines instead of exiting into the product catch pot.

Appendix

D.

D.1 GC product analysis

The peak identification which was done by Nagooroo, (2011) was used as a basis. In the case whereby the pure compound was available, a reference mixture was made to identify the peak. To make these reference mixtures, the product sample was spiked with the pure compound. The chromatogram of the reference mixture was then compared to the original product sample chromatogram to determine the various unknown peaks. The remaining peaks were identified by GCMS (Nagooroo, 2011).

Table D.1 gives a summary of the method used to identify the respective peaks. The GC column used in this study was the same type of column used by Nagooroo, (2011) but not identical in retention times. To compensate for the different retention times, a product sample produced by Nagooroo, (2011) was used as a reference to determine the peaks in this study. A typical GC chromatogram is shown Figure D.2 with subsequent enlarged figures to follow indicating the respective peaks.

Table D.1: Peak identification of gas chromatograms for Varian CP-4800 GC (Nagooroo, 2011).

Peak	Compound	Method
	Acetone	Pure compound reference
1	Isopropyl-Tolyl Ether	GCMS
2	Phenol	Pure compound reference
3	*o*-Cresol	Pure compound reference
4	*p*-Cresol	Pure compound reference
5	*m*-Cresol	Pure compound reference
6	2,4-Xylenol	Pure compound reference
7	2,5-Xylenol	Pure compound reference
8	2,3-Xylenol	Pure compound reference
9	2-Isopropyl- 4-Methyl Phenol	GCMS
10	2-Isopropyl-3-Methyl Phenol	GCMS
11	6-Isopropyl-3-Methyl Phenol (Thymol)	Pure compound reference
12	6-n-Propyl-3-Methyl Phenol	GCMS
13	2,6-Diisopropyl-3-Methyl Phenol	GCMS
14	5-Isopropyl-3-Methyl Phenol	Pure compound reference
15	4-Isopropyl-3-Methyl Phenol	Pure compound reference
16	4,6-Diisopropyl-3-Methyl Phenol	GCMS
17	5,6-Diisopropyl-3-Methyl Phenol	GCMS
18	Heavies	GCMS

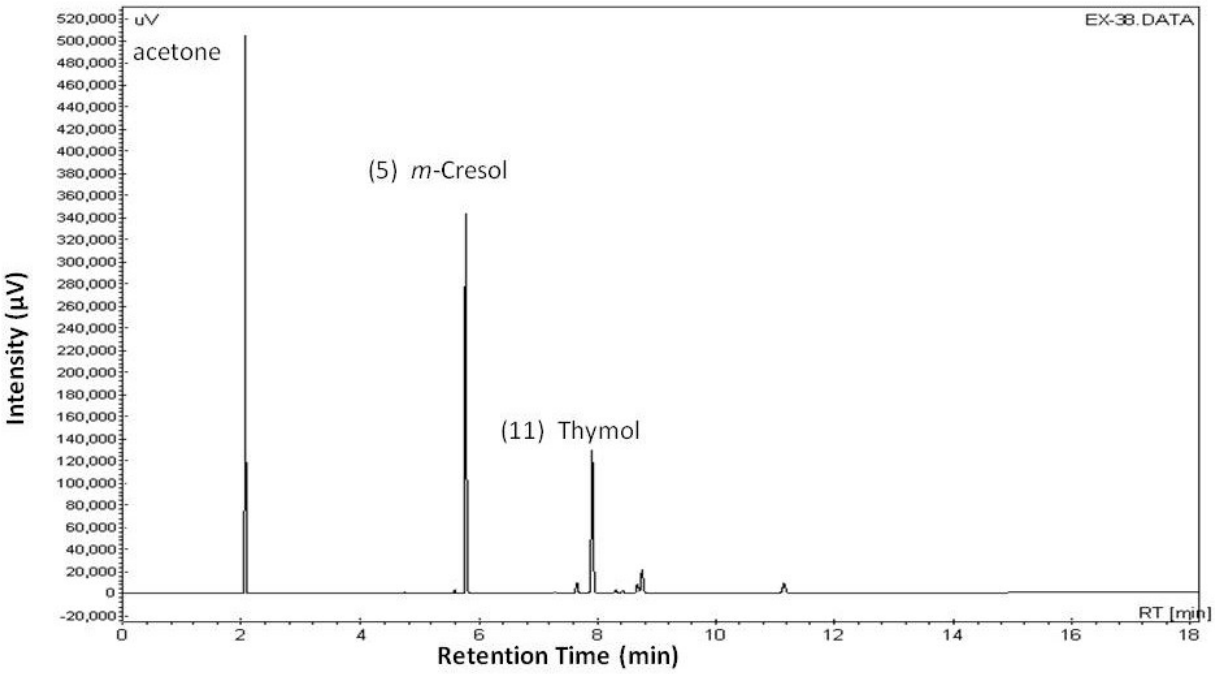

Figure D.1: Typical chromatogram of a product sample from the fixed-bed configuration for the conversion of m-Cresol and isopropanol (1:1 molar ratio) at standard conditions using the Varian 4800 GC.

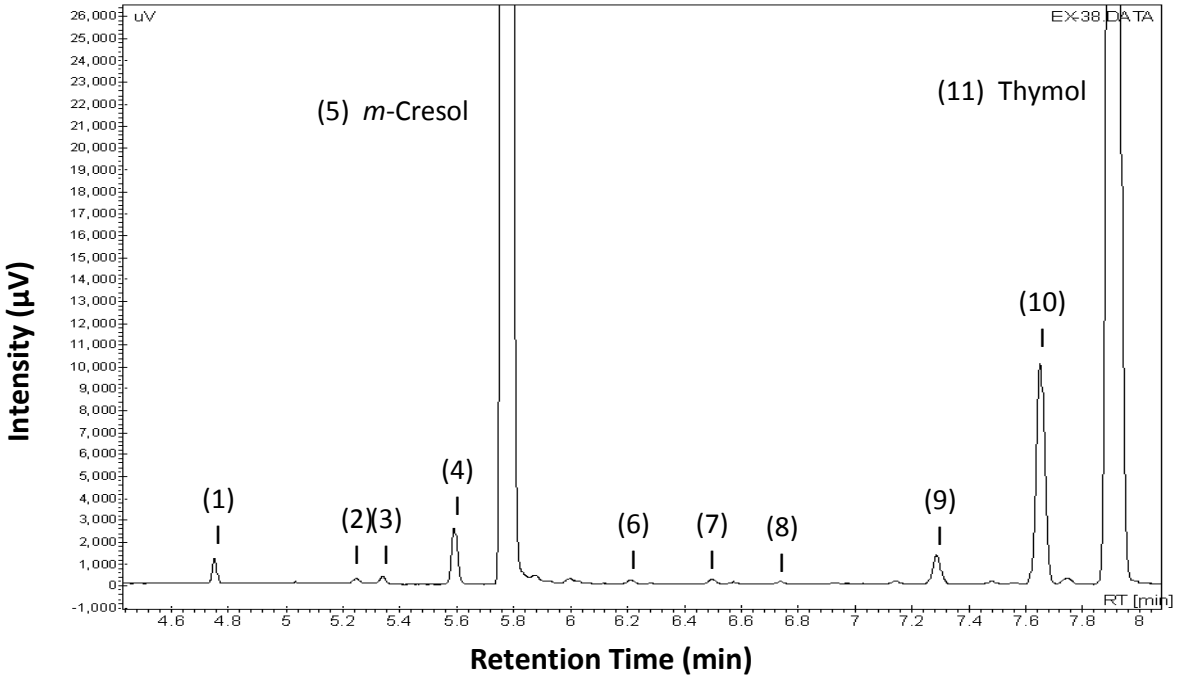

Figure D.2: Typical gas chromatogram of product sample from retention time of 4.4 to 8.1 minutes using the Varian 4800 GC.

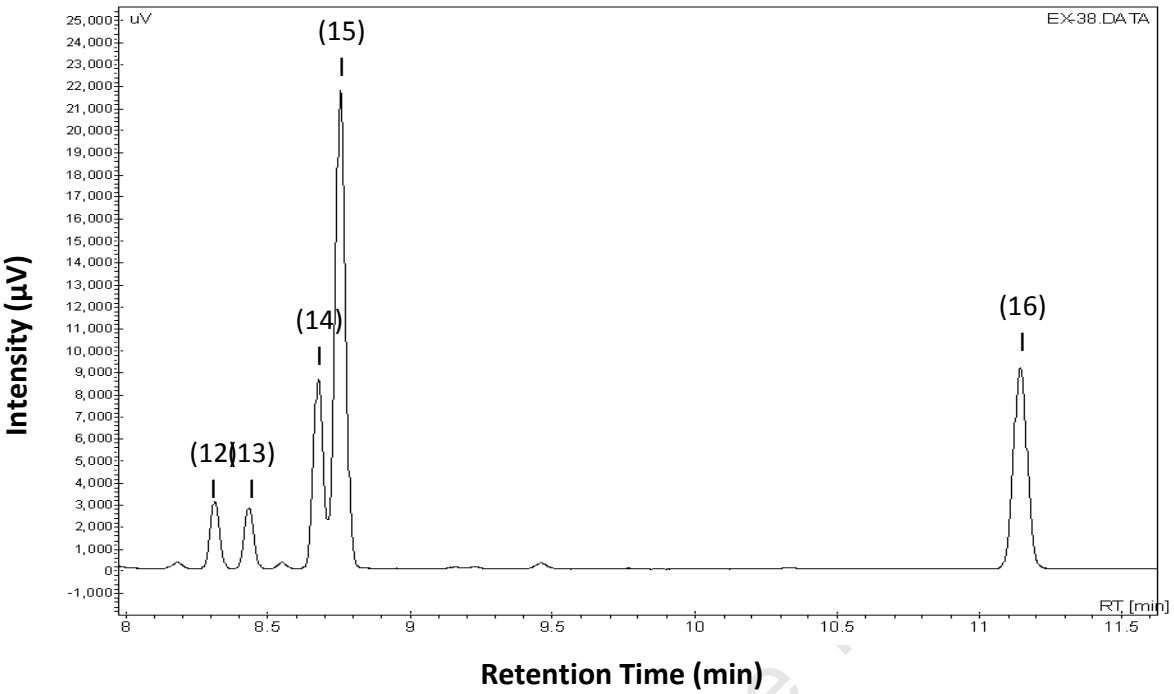

Figure D.3: Typical gas chromatogram of product sample from retention time of 8 to 11.6 minutes using the Varian 4800 GC.

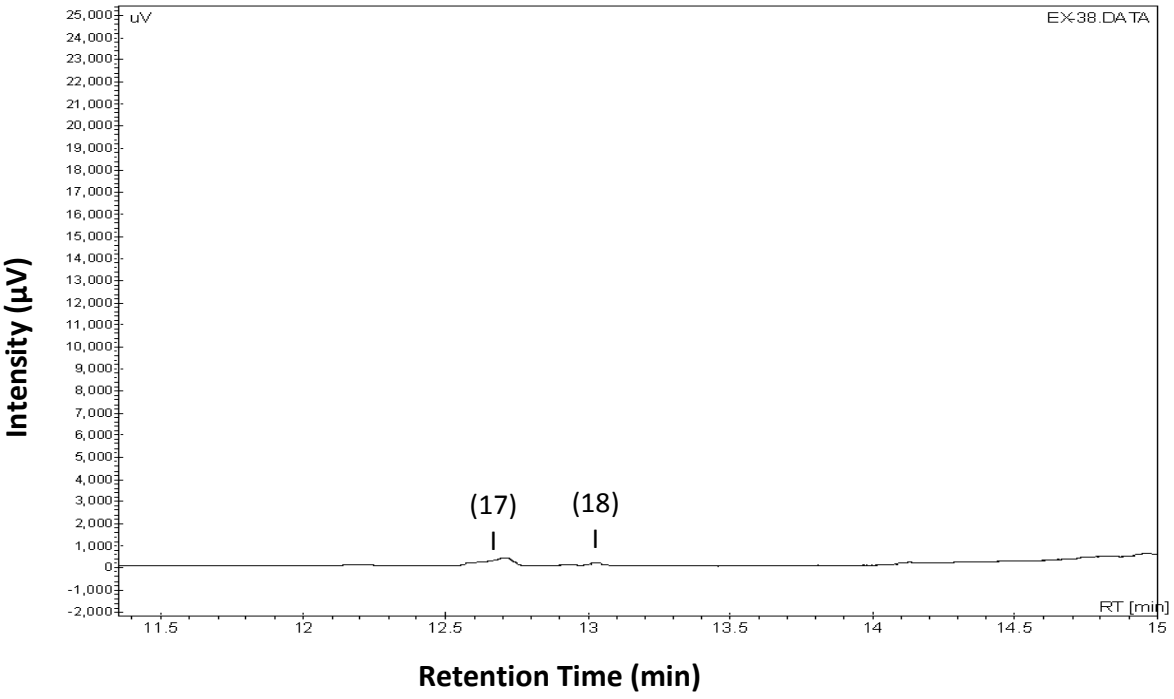

Figure D.4: Typical gas chromatogram of product sample from retention time of 11.4 to 15 minutes using the Varian 4800 GC.

Appendix

E.

E.1 Calculation of WHSV for various catalysts

The pump flow rate required to give identical WHSV was calculated based on the amount of zeolite present in the catalyst. Table E.1 gives a summary the pump flow rate required for the respective catalysts and WHSV required. The WHSV was based on a feed density of 0.902 g/ml (determined experimentally).

Table E.1: Summary of pump flow rates required for different catalysts at the same WHSV

Zeolite type	H-MFI-90 extrudates	H-MFI-90 powder	Simulated Washcoat	Microchannel reactor C
Total catalyst added	5.83	5.83	5.83	0.0251
Zeolite(%)	80	100	75	75
Zeolite amount	4.66	5.83	4.37	0.0188
Pump (ml/min)	0.16	0.16	0.16	0.0005
WHSV ($g_{feed}/g_{zeolite}h$)	1.2	0.96	1.28	0.93
Pump (ml/min)	0.04	0.05	0.037	-
WHSV ($g_{feed}/g_{zeolite}h$)	0.3	0.3	0.3	-
Pump (ml/min)	0.32	0.302	0.227	0.001
WHSV ($g_{feed}/g_{zeolite}h$)	2.4	1.81	1.81	1.85
Pump (ml/min)	0.64	0.604	0.454	0.002
WHSV ($g_{feed}/g_{zeolite}h$)	4.8	3.62	3.63	3.71

E.2 Experimental data

In this section the conversion, selectivity, and yield of the respective compounds is given at steady state and the first 100 hours where the initial deactivation occurred. The experimental runs conducted in the fixed-bed reactor were for the H-MFI-90 extrudates, H-MFI-90 powder, simulated washcoating and H-MFI-90 powder repeat catalysts, as well as in the microreactor configuration (75% Zeolite washcoating).

Table E.2: Conversion, selectivity and yield data for H-MFI-90 extrudates

EXTRUDATE	EX-1	EX-2	EX-3	EX-4	EX-5	EX-6	EX-7	EX-8	EX-9	EX-10	EX-11	EX-12	EX-13	EX-14
Time on Stream	1:22:38	2:22:48	7:26:48	9:26:48	11:30:48	13:27:48	18:08:48	30:30:48	37:20:48	57:55:46	67:10:46	77:10:46	80:09:46	83:05:44
Entry Temperature	90	90	91	91	92	93	93	93	92	91	93	93	86	93
Temperature	275	275	275	274	275	274	275	275	275	275	274	275	275	276
WHSV	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	24.44	40.75	51.03	51.44	53.36	50.32	48.65	45.32	44.65	36.57	35.10	35.57	34.20	33.82
Thymol Selectivity	4.16	42.49	53.41	59.46	60.10	61.68	62.86	64.13	64.23	66.43	66.14	65.67	67.32	67.02
Thymol Yield	1.02	17.32	27.25	30.58	32.07	31.04	30.58	29.07	28.68	24.30	23.21	23.36	23.02	22.66
S3-isopropyl-5-methylphenol	**19.36**	**15.42**	**12.49**	**10.06**	**9.27**	**8.57**	**7.74**	**6.85**	**6.14**	**5.47**	**5.58**	**4.91**	**4.73**	**4.73**
Y3-methyl-5-isopropylphenol	4.73	6.28	6.37	5.17	4.95	4.31	3.77	3.10	2.74	2.00	1.96	1.75	1.62	1.60
S4-isopropyl-3-methylphenol	**6.32**	**6.48**	**8.06**	**8.81**	**9.15**	**8.88**	**9.24**	**9.27**	**10.06**	**10.10**	**9.70**	**9.83**	**10.04**	**10.00**
Y3-methyl-4-isopropylphenol	1.54	2.64	4.11	4.53	4.88	4.47	4.50	4.20	4.49	3.70	3.40	3.50	3.43	3.38
S2-isopropyl-3-methylphenol	**1.11**	**0.85**	**1.26**	**1.87**	**2.17**	**2.39**	**2.85**	**3.45**	**4.04**	**4.57**	**4.83**	**4.87**	**5.40**	**5.40**
Y3-methyl-2-isopropylphenol	0.27	0.35	0.64	0.96	1.16	1.20	1.38	1.56	1.80	1.67	1.70	1.73	1.85	1.83
Thymol	13.45	65.13	71.01	74.13	74.48	75.66	76.02	76.61	76.04	76.73	76.68	77.00	76.95	76.90
3-methyl-5-isopropylphenol	62.55	23.63	16.61	12.54	11.49	10.51	9.36	8.18	7.27	6.31	6.47	5.75	5.41	5.42
3-methyl-2-isopropylphenol	20.42	9.93	10.71	10.99	11.34	10.89	11.18	11.08	11.91	11.67	11.25	11.53	11.47	11.48
3-methyl-4-isopropylphenol	3.58	1.30	1.67	2.34	2.69	2.94	3.44	4.12	4.78	5.28	5.60	5.72	6.17	6.20
STotal.Isomer	**30.95**	**65.24**	**75.22**	**80.20**	**80.70**	**81.52**	**82.69**	**83.70**	**84.47**	**86.57**	**86.25**	**85.28**	**87.48**	**87.16**
YTotal.Isomer	7.56	26.58	38.38	41.25	43.06	41.02	40.23	37.94	37.71	31.66	30.27	30.34	29.92	29.47
Slights	9.70	4.06	1.87	1.44	1.28	1.30	1.24	1.21	1.17	1.16	1.23	1.19	1.13	1.18
Ylights	2.37	1.65	0.95	0.74	0.68	0.65	0.60	0.55	0.52	0.42	0.43	0.42	0.39	0.40
SC-10	18.01	9.65	6.03	4.54	4.06	3.90	3.30	2.85	2.35	2.30	2.22	3.78	1.84	1.85
YC-10	4.40	3.93	3.08	2.34	2.17	1.96	1.61	1.29	1.05	0.84	0.78	1.34	0.63	0.63
Sdi-isopropylated	5.89	5.66	9.34	9.37	10.40	9.38	9.84	9.57	9.56	7.41	7.49	7.17	7.01	7.15
Ydi-isopropylated	1.44	2.31	4.76	4.82	5.55	4.72	4.79	4.34	4.27	2.71	2.63	2.55	2.40	2.42
Sheavies	0.44	2.09	1.07	0.65	0.52	0.91	0.29	0.26	0.18	0.13	0.24	0.14	0.10	0.17
Yheavies	0.11	0.85	0.55	0.34	0.28	0.46	0.14	0.12	0.08	0.05	0.08	0.05	0.03	0.06
Sether	1.41	0.24	0.11	0.13	0.15	0.20	0.20	0.26	0.31	0.33	0.40	0.39	0.41	0.44
Yether	0.34	0.10	0.06	0.06	0.08	0.10	0.10	0.12	0.14	0.12	0.14	0.14	0.14	0.15

Table E.3: Conversion, selectivity and yield data for H-MFI-90 extrudates (cont.)

EXTRUDATE	EX-15	EX-16	EX-17	EX-18	EX-19	EX-20	EX-21	EX-22	EX-23	EX-24	EX-25	EX-26	EX-27	EX-28	EX-29
Time on Stream	115:13:44	117:12:44	119:12:44	121:13:44	125:06:44	144:01:44	146:23:44	150:07:44	159:10:44	161:09:44	171:12:44	172:05:44	173:19:44	174:08:44	174:34:44
Entry Temperature	94	94	94	94	92	92	93	93	93	92	94	96	96	95	95
Temperature	275	275	275	275	275	275	276	275	275	276	275	274	274	275	275
WHSV	0.6	0.6	0.6	0.6	0.6	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.08	0.08	0.08	0.08	0.08	0.04	0.04	0.04	0.04	0.04	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	42.74	40.52	40.26	42.99	42.06	46.87	46.73	48.04	48.24	47.12	28.00	29.07	27.18	26.17	25.73
Thymol Selectivity	67.52	67.22	67.11	67.03	66.42	62.13	62.02	62.29	62.27	61.71	67.29	66.64	67.21	67.07	67.38
Thymol Yield	28.86	27.24	27.02	28.82	27.93	29.12	28.98	29.92	30.04	29.08	18.84	19.37	18.27	17.55	17.33
S3-isopropyl-5-methylphenol	**7.01**	**7.38**	**7.09**	**6.85**	**7.36**	**11.86**	**12.04**	**11.86**	**11.71**	**11.46**	**3.98**	**4.01**	**3.77**	**3.59**	**3.53**
Y3-methyl-5-isopropylphenol	3.00	2.99	2.86	2.95	3.09	5.56	5.63	5.70	5.65	5.40	1.11	1.16	1.03	0.94	0.91
S4-isopropyl-3-methylphenol	**8.99**	**9.07**	**8.80**	**8.93**	**9.28**	**7.59**	**7.70**	**7.72**	**7.82**	**7.69**	**10.00**	**10.32**	**10.03**	**10.00**	**9.98**
Y3-methyl-4-isopropylphenol	3.84	3.68	3.54	3.84	3.90	3.56	3.60	3.71	3.77	3.62	2.80	3.00	2.73	2.62	2.57
S2-isopropyl-3-methylphenol	**2.70**	**2.61**	**3.00**	**2.88**	**2.79**	**1.59**	**1.57**	**1.50**	**1.55**	**1.66**	**6.75**	**6.75**	**7.22**	**7.75**	**7.94**
Y3-methyl-2-isopropylphenol	1.15	1.06	1.21	1.24	1.17	0.75	0.73	0.72	0.75	0.78	1.89	1.96	1.96	2.03	2.04
Thymol	78.31	77.91	78.03	78.22	77.37	74.69	74.43	74.71	74.70	74.78	76.45	75.98	76.17	75.87	75.85
3-methyl-5-isopropylphenol	8.13	8.55	8.25	7.99	8.57	14.26	14.45	14.23	14.05	13.89	4.52	4.57	4.27	4.06	3.97
3-methyl-2-isopropylphenol	10.43	10.52	10.23	10.42	10.81	9.13	9.24	9.26	9.38	9.32	11.36	11.76	11.37	11.31	11.24
3-methyl-4-isopropylphenol	3.13	3.02	3.49	3.36	3.25	1.92	1.88	1.80	1.86	2.01	7.67	7.69	8.18	8.77	8.94
STotal.Isomer	**86.22**	**86.27**	**86.01**	**85.70**	**85.84**	**83.18**	**83.33**	**83.37**	**83.35**	**82.52**	**88.02**	**87.71**	**88.23**	**88.41**	**88.83**
YTotal.Isomer	36.85	34.96	34.63	36.84	36.10	38.99	38.94	40.05	40.21	38.88	24.65	25.50	23.98	23.14	22.85
Slights	1.21	1.13	1.19	1.09	1.18	1.54	1.57	1.44	1.56	1.45	1.26	1.27	1.23	1.14	1.30
Ylights	0.52	0.46	0.48	0.47	0.50	0.72	0.73	0.69	0.75	0.68	0.35	0.37	0.33	0.30	0.33
SC-10	2.58	2.73	2.74	2.62	2.73	4.41	4.35	4.23	4.22	4.27	1.74	1.73	1.62	1.41	1.36
YC-10	1.10	1.11	1.10	1.13	1.15	2.07	2.03	2.03	2.03	2.01	0.49	0.50	0.44	0.37	0.35
Sdi-isopropylated	7.82	7.56	7.60	8.13	7.92	7.65	7.50	8.06	7.90	8.13	5.84	6.26	5.76	5.57	5.34
Ydi-isopropylated	3.34	3.07	3.06	3.50	3.33	3.59	3.51	3.87	3.81	3.83	1.64	1.82	1.57	1.46	1.37
Sheavies	0.07	0.07	0.12	0.21	0.09	0.32	0.31	0.13	0.18	0.51	0.26	0.20	0.18	0.48	0.18
Yheavies	0.03	0.03	0.05	0.09	0.04	0.15	0.15	0.06	0.09	0.24	0.07	0.06	0.05	0.13	0.05
Sether	0.20	0.20	0.25	0.27	0.21	0.13	0.12	0.11	0.15	0.09	0.56	0.56	0.57	0.58	0.78
Yether	0.08	0.08	0.10	0.12	0.09	0.06	0.06	0.05	0.07	0.04	0.16	0.16	0.16	0.15	0.20

Table E.4: Conversion, selectivity and yield data for H-MFI-90 extrudates (cont.)

EXTRUDATE	EX-30	EX-31	EX-32	EX-33	EX-34	EX-35	EX-36	EX-37	EX-38	EX-39	EX-40	EX-41	EX-42	EX-43
Time on Stream	176:10:44	177:03:44	179:00:44	179:24:44	180:01:44	181:30:44	181:58:44	182:25:44	183:55:44	199:04:44	200:04:44	201:55:44	202:32:44	203:44:44
Entry Temperature	89	89	90	89	90	90	90	90	90	85	85	93	94	95
Temperature	275	276	276	275	276	275	275	274	275	275	275	275	275	275
WHSV	2.4	2.4	2.4	2.4	2.4	4.79	4.79	4.79	4.79	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.32	0.32	0.32	0.32	0.32	0.64	0.64	0.64	0.64	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	18.92	19.21	19.39	19.00	18.99	11.01	11.15	11.37	11.75	25.53	27.10	26.53	25.15	25.50
Thymol Selectivity	62.27	62.93	62.44	62.52	62.34	53.57	53.61	53.23	52.46	67.70	67.51	66.38	67.53	67.46
Thymol Yield	11.78	12.09	12.11	11.88	11.84	5.90	5.98	6.05	6.17	17.29	18.30	17.61	16.98	17.20
S3-isopropyl-5-methylphenol	**2.54**	**2.34**	**2.39**	**2.23**	**2.10**	**1.56**	**1.49**	**1.46**	**1.43**	**2.34**	**2.41**	**2.33**	**2.27**	**2.25**
Y3-methyl-5-isopropylphenol	0.48	0.45	0.46	0.42	0.40	0.17	0.17	0.17	0.17	0.60	0.65	0.62	0.57	0.57
S4-isopropyl-3-methylphenol	**9.49**	**9.30**	**9.51**	**8.70**	**8.87**	**7.95**	**7.79**	**7.61**	**7.32**	**8.04**	**8.31**	**7.83**	**7.66**	**7.88**
Y3-methyl-4-isopropylphenol	1.79	1.79	1.84	1.65	1.69	0.88	0.87	0.87	0.86	2.05	2.25	2.08	1.93	2.01
S2-isopropyl-3-methylphenol	**14.34**	**14.37**	**14.43**	**15.15**	**15.43**	**22.18**	**22.52**	**22.81**	**23.17**	**11.45**	**10.98**	**11.61**	**11.82**	**11.59**
Y3-methyl-2-isopropylphenol	2.71	2.76	2.80	2.88	2.93	2.44	2.51	2.59	2.72	2.92	2.98	3.08	2.97	2.95
Thymol	70.25	70.75	70.33	70.57	70.25	62.83	62.77	62.54	62.18	75.61	75.67	75.30	75.64	75.64
3-methyl-5-isopropylphenol	2.87	2.63	2.70	2.52	2.37	1.83	1.74	1.71	1.69	2.62	2.70	2.64	2.54	2.53
3-methyl-2-isopropylphenol	10.70	10.46	10.72	9.82	10.00	9.33	9.12	8.95	8.68	8.98	9.31	8.88	8.58	8.84
3-methyl-4-isopropylphenol	16.18	16.16	16.25	17.09	17.39	26.01	26.37	26.80	27.46	12.79	12.31	13.17	13.24	12.99
STotal.Isomer	**88.64**	**88.95**	**88.78**	**88.60**	**88.74**	**85.26**	**85.41**	**85.11**	**84.38**	**89.54**	**89.22**	**88.16**	**89.28**	**89.18**
YTotal.Isomer	16.77	17.08	17.21	16.83	16.85	9.39	9.52	9.68	9.92	22.86	24.18	23.38	22.45	22.74
Slights	1.28	1.29	1.29	1.40	1.49	1.57	1.60	1.53	1.51	1.24	1.24	1.43	1.24	1.30
Ylights	0.24	0.25	0.25	0.27	0.28	0.17	0.18	0.17	0.18	0.32	0.33	0.38	0.31	0.33
SC-10	0.95	0.92	0.88	0.86	0.75	0.47	0.43	0.43	0.29	0.75	0.74	0.78	0.74	0.75
YC-10	0.18	0.18	0.17	0.16	0.14	0.05	0.05	0.05	0.03	0.19	0.20	0.21	0.18	0.19
Sdi-isopropylated	4.42	4.21	4.62	4.42	4.50	2.87	2.71	2.82	2.94	5.43	5.99	6.15	5.48	5.67
Ydi-isopropylated	0.84	0.81	0.89	0.84	0.85	0.32	0.30	0.32	0.35	1.39	1.62	1.63	1.38	1.44
Sheavies	0.26	0.30	0.17	0.29	0.22	0.40	0.34	0.31	0.56	0.12	0.14	0.39	0.17	0.19
Yheavies	0.05	0.06	0.03	0.05	0.04	0.04	0.04	0.04	0.07	0.03	0.04	0.10	0.04	0.05
Sether	1.24	1.21	1.16	1.25	1.46	3.80	4.08	4.38	4.96	0.76	0.68	0.90	0.88	0.80
Yether	0.23	0.23	0.22	0.24	0.28	0.42	0.46	0.50	0.58	0.20	0.18	0.24	0.22	0.20

Table E.5: Conversion, selectivity and yield data for simulated washcoating

	WC-1	WC-2	WC-3	WC-4	WC-5	WC-6	WC-7	WC-8	WC-9	WC-10
Time on Stream	07:10:44	08:10:44	09:00:44	11:00:44	11:50:44	14:30:44	17:30:44	31:40:44	33:00:44	35:00:44
Entry Temperature	103	103	104	105	105	105	105	101	104	103
Temperature	274	277	278	276	275	275	275	275	275	275
$WHSV_{Wet}$	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guage Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	24.62	43.91	46.10	46.13	43.63	41.12	39.79	34.70	32.55	31.69
Thymol Selectivity	51.51	62.78	63.38	53.81	62.92	64.04	63.33	63.20	63.43	63.12
Thymol Yield	12.68	27.56	29.22	24.82	27.45	26.33	25.20	21.93	20.65	20.01
S3-isopropyl-5-methylphenol	**7.83**	**6.09**	**5.84**	**4.32**	**5.15**	**4.97**	**4.68**	**4.09**	**3.90**	**3.91**
Y3-methyl-5-isopropylphenol	1.93	2.68	2.69	1.99	2.24	2.04	1.86	1.42	1.27	1.24
S4-isopropyl-3-methylphenol	**8.30**	**10.21**	**10.18**	**8.97**	**10.99**	**10.96**	**11.26**	**11.52**	**11.33**	**11.36**
Y3-methyl-4-isopropylphenol	2.04	4.48	4.69	4.14	4.80	4.51	4.48	4.00	3.69	3.60
S2-isopropyl-3-methylphenol	**1.91**	**3.13**	**3.20**	**3.40**	**4.15**	**4.47**	**4.97**	**6.06**	**6.47**	**7.12**
Y3-methyl-2-isopropylphenol	0.47	1.37	1.47	1.57	1.81	1.84	1.98	2.10	2.11	2.26
Thymol	74.06	76.36	76.74	76.32	75.62	75.84	75.18	74.47	74.51	73.82
3-methyl-5-isopropylphenol	11.26	7.41	7.07	6.13	6.18	5.88	5.55	4.82	4.58	4.57
3-methyl-2-isopropylphenol	11.93	12.42	12.33	12.73	13.21	12.98	13.37	13.57	13.30	13.29
3-methyl-4-isopropylphenol	2.75	3.81	3.87	4.83	4.99	5.29	5.90	7.14	7.60	8.32
STotal.Isomer	**69.55**	**82.21**	**82.59**	**70.51**	**83.21**	**84.44**	**84.24**	**84.87**	**85.14**	**85.51**
YTotal.Isomer	17.13	36.10	38.07	32.53	36.30	34.72	33.52	29.45	27.71	27.10
Slights	2.20	1.52	1.53	1.07	1.18	1.25	1.28	1.55	1.28	1.22
Ylights	0.54	0.67	0.71	0.49	0.52	0.51	0.51	0.54	0.42	0.39
SC-10	7.25	3.03	2.98	17.83	2.26	2.17	1.93	1.73	1.48	1.38
YC-10	1.79	1.33	1.38	8.23	0.99	0.89	0.77	0.60	0.48	0.44
Sdi-isopropylated	6.28	8.66	8.50	6.68	8.76	7.80	7.86	6.76	6.93	6.61
Ydi-isopropylated	1.55	3.80	3.92	3.08	3.82	3.21	3.13	2.34	2.26	2.09
Sheavies	4.48	1.65	1.57	1.12	1.25	1.06	1.10	0.98	0.88	0.87
Yheavies	1.10	0.72	0.72	0.52	0.55	0.44	0.44	0.34	0.29	0.28
Sether	0.38	0.30	0.29	0.30	0.34	0.31	0.41	0.53	0.60	0.66
Yether	0.09	0.13	0.13	0.14	0.15	0.13	0.16	0.18	0.20	0.21

Table E.6: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-11	WC-12	WC-13	WC-14	WC-15	WC-16	WC-17	WC-18	WC-19	WC-20
Time on Stream	37:00:44	42:54:44	55:00:44	62:00:44	64:00:44	66:00:44	76:00:44	78:00:44	80:00:44	82:00:44
Entry Temperature	101	103	100	102	105	105	99	102	101	101
Temperature	275	275	275	276	275	275	275	275	275	275
WHSV	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	28.51	30.25	27.10	26.65	24.68	25.26	23.06	24.47	22.83	23.06
Thymol Selectivity	64.05	62.89	62.60	61.39	63.29	60.62	61.69	60.48	61.06	60.90
Thymol Yield	18.26	19.02	16.96	16.36	15.62	15.31	14.22	14.80	13.94	14.04
S3-isopropyl-5-methylphenol	**3.49**	**3.54**	**3.13**	**2.98**	**2.90**	**2.90**	**2.83**	**14.63**	**2.63**	**2.64**
Y3-methyl-5-isopropylphenol	0.99	1.07	0.85	0.79	0.72	0.73	0.68	0.70	0.60	0.61
S4-isopropyl-3-methylphenol	**10.94**	**11.53**	**11.21**	**11.57**	**11.05**	**11.41**	**11.38**	**11.32**	**11.20**	**11.30**
Y3-methyl-4-isopropylphenol	3.12	3.49	3.04	3.08	2.73	2.88	2.76	2.67	2.56	2.61
S2-isopropyl-3-methylphenol	**7.83**	**8.01**	**9.36**	**9.61**	**9.96**	**10.76**	**11.40**	**11.53**	**11.90**	**11.91**
Y3-methyl-2-isopropylphenol	2.23	2.42	2.54	2.56	2.46	2.72	2.63	2.82	2.72	2.75
Thymol	74.21	73.16	72.53	71.76	72.58	70.75	71.01	69.81	70.34	70.21
3-methyl-5-isopropylphenol	4.04	4.12	3.63	3.49	3.33	3.38	3.28	3.19	3.04	3.05
3-methyl-2-isopropylphenol	12.68	13.41	12.99	13.52	12.67	13.32	13.39	13.12	12.91	13.02
3-methyl-4-isopropylphenol	9.07	9.32	10.85	11.23	11.42	12.55	13.12	13.31	13.71	13.72
STotal.Isomer	**86.31**	**85.97**	**86.31**	**85.56**	**87.21**	**85.68**	**86.88**	**86.64**	**86.81**	**86.75**
YTotal.Isomer	24.61	26.00	23.39	22.80	21.53	21.64	20.03	21.20	19.82	20.00
Slights	1.31	1.24	1.33	1.31	1.24	1.23	1.32	1.37	1.26	1.43
Ylights	0.37	0.38	0.36	0.35	0.31	0.31	0.30	0.33	0.29	0.33
SC-10	1.22	1.16	0.97	0.89	0.89	0.77	0.76	0.75	0.72	0.70
YC-10	0.35	0.35	0.26	0.24	0.22	0.20	0.18	0.18	0.16	0.16
Sdi-isopropylated	5.88	6.36	5.51	6.12	4.94	5.91	4.81	4.92	4.96	4.89
Ydi-isopropylated	1.68	1.92	1.49	1.63	1.22	1.49	1.11	1.20	1.13	1.13
Sheavies	0.53	0.70	0.85	0.85	0.57	0.74	0.67	0.80	0.66	0.77
Yheavies	0.15	0.21	0.23	0.23	0.14	0.19	0.15	0.20	0.15	0.18
Sether	0.77	0.72	0.88	0.93	0.91	1.07	1.05	1.07	1.05	1.00
Yether	0.22	0.22	0.24	0.25	0.22	0.27	0.24	0.26	0.24	0.23

Table E.7: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-21	WC-22	WC-23	WC-24	WC-25	WC-26	WC-27	WC-28	WC-29	WC-30	WC-31	WC-32
Time on Stream	84:00:44	85:50:44	101:00:44	102:00:44	103:00:11	104:01:34	113:00:34	127:59:34	129:01:34	130:01:34	131:01:34	131:47:34
Entry Temperature	100	102	101	101	101	105	88	89	90	90	90	90
Temperature	275	275	275	275	275	275	275	275	275	275	274	275
WHSV	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.2	1.2	1.2	1.2	1.2
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.15	0.15	0.15	0.15
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	22.22	22.41	19.64	20.17	19.27	16.01	19.48	19.65	18.80	19.17	18.60	18.65
Thymol Selectivity	60.84	60.69	59.97	59.43	59.19	59.52	61.51	57.56	58.38	58.24	57.53	57.94
Thymol Yield	13.52	13.60	11.78	11.99	11.40	9.53	11.98	11.31	10.97	11.16	10.70	10.81
S3-isopropyl-5-methylphenol	**2.60**	**2.61**	**2.40**	**2.36**	**2.38**	**2.32**	**2.26**	**2.04**	**2.06**	**2.02**	**1.98**	**2.03**
Y3-methyl-5-isopropylphenol	0.58	0.59	0.47	0.48	0.46	0.37	0.44	0.40	0.39	0.39	0.37	0.38
S4-isopropyl-3-methylphenol	**11.18**	**11.19**	**10.87**	**10.93**	**10.96**	**10.78**	**10.16**	**10.42**	**10.28**	**10.69**	**10.55**	**10.60**
Y3-methyl-4-isopropylphenol	2.48	2.51	2.13	2.20	2.11	1.73	1.98	2.05	1.93	2.05	1.96	1.98
S2-isopropyl-3-methylphenol	**12.14**	**12.11**	**14.21**	**14.39**	**14.16**	**14.47**	**13.87**	**15.94**	**16.58**	**16.35**	**16.50**	**16.57**
Y3-methyl-2-isopropylphenol	2.70	2.71	2.79	2.90	2.73	2.32	2.70	3.13	3.12	3.13	3.07	3.09
Thymol	70.12	70.08	68.58	68.23	68.28	68.34	70.05	66.96	66.87	66.71	66.46	66.49
3-methyl-5-isopropylphenol	3.00	3.02	2.75	2.71	2.75	2.67	2.58	2.37	2.36	2.32	2.29	2.33
3-methyl-2-isopropylphenol	12.89	12.92	12.43	12.54	12.65	12.38	11.57	12.13	11.78	12.24	12.19	12.16
3-methyl-4-isopropylphenol	13.99	13.98	16.25	16.52	16.33	16.62	15.80	18.54	18.99	18.73	19.06	19.02
STotal.Isomer	**86.76**	**86.61**	**87.45**	**87.10**	**86.70**	**87.10**	**87.80**	**85.96**	**87.31**	**87.30**	**86.57**	**87.15**
YTotal.Isomer	19.27	19.41	17.17	17.57	16.70	13.95	17.10	16.89	16.41	16.74	16.10	16.25
Slights	1.32	1.09	1.17	1.26	1.27	1.30	1.49	2.42	1.19	1.15	1.36	1.31
Ylights	0.29	0.24	0.23	0.25	0.25	0.21	0.29	0.47	0.22	0.22	0.25	0.24
SC-10	0.70	0.71	0.46	0.45	0.46	0.43	0.50	0.42	0.31	0.33	0.29	0.31
YC-10	0.16	0.16	0.09	0.09	0.09	0.07	0.10	0.08	0.06	0.06	0.05	0.06
Sdi-isopropylated	4.79	4.88	4.15	4.30	4.39	4.03	3.90	4.07	3.90	4.05	3.99	4.00
Ydi-isopropylated	1.06	1.09	0.81	0.87	0.84	0.65	0.76	0.80	0.73	0.78	0.74	0.75
Sheavies	0.75	0.92	0.44	0.61	0.66	0.62	0.48	0.74	0.65	0.56	1.15	0.38
Yheavies	0.17	0.21	0.09	0.12	0.13	0.10	0.09	0.14	0.12	0.11	0.21	0.07
Sether	1.08	1.14	1.39	1.34	1.41	1.21	0.96	1.24	1.40	1.34	1.42	1.22
Yether	0.24	0.26	0.27	0.27	0.27	0.19	0.19	0.24	0.26	0.26	0.26	0.23

Table E.8: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-33	WC-34	WC-35	WC-36	WC-37	WC-38	WC-39	WC-40	WC-41	WC-42	WC-43
Time on Stream	172:01:34	174:01:34	176:01:34	178:01:34	179:57:34	183:55:37	193:01:37	194:01:37	195:01:37	196:01:37	196:59:37
Entry Temperature	92	93	94	94	94	93	90	91	91	89	88
Temperature	274	274	274	274	275	276	275	275	275	275	275
WHSV	0.3	0.3	0.3	0.3	0.3	0.3	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)	0.037	0.037	0.037	0.037	0.037	0.037	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3
Conversion	39.43	42.60	45.03	38.70	37.40	36.22	19.33	18.08	17.73	18.02	15.67
Thymol Selectivity	65.05	65.42	64.61	64.06	65.86	63.97	57.76	57.31	57.78	57.18	57.07
Thymol Yield	25.65	27.87	29.09	24.79	24.63	23.17	11.17	10.36	10.24	10.31	8.94
S3-isopropyl-5-methylphenol	**4.91**	**4.69**	**4.84**	**4.76**	**4.57**	**5.19**	**2.24**	**2.09**	**2.08**	**2.07**	**1.81**
Y3-methyl-5-isopropylphenol	1.93	2.00	2.18	1.84	1.71	1.88	0.43	0.38	0.37	0.37	0.28
S4-isopropyl-3-methylphenol	**9.53**	**9.32**	**9.34**	**9.76**	**9.61**	**9.37**	**11.06**	**10.65**	**10.66**	**10.98**	**10.19**
Y3-methyl-4-isopropylphenol	3.76	3.97	4.21	3.78	3.59	3.39	2.14	1.92	1.89	1.98	1.60
S2-isopropyl-3-methylphenol	**5.05**	**4.91**	**4.42**	**4.81**	**5.03**	**5.54**	**15.84**	**16.65**	**16.66**	**16.90**	**18.10**
Y3-methyl-2-isopropylphenol	1.99	2.09	1.99	1.86	1.88	2.00	3.06	3.01	2.95	3.05	2.84
Thymol	76.95	77.56	77.65	76.82	77.42	76.09	66.47	66.11	66.28	65.62	65.48
3-methyl-5-isopropylphenol	5.80	5.56	5.82	5.71	5.37	6.18	2.57	2.41	2.38	2.38	2.07
3-methyl-2-isopropylphenol	11.28	11.06	11.22	11.71	11.29	11.15	12.72	12.28	12.22	12.60	11.68
3-methyl-4-isopropylphenol	5.97	5.83	5.31	5.77	5.92	6.58	18.23	19.20	19.11	19.40	20.76
STotal.Isomer	**84.54**	**84.35**	**83.21**	**83.39**	**85.07**	**84.07**	**86.90**	**86.69**	**87.17**	**87.14**	**87.16**
YTotal.Isomer	33.33	35.93	37.47	32.27	31.82	30.45	16.80	15.67	15.46	15.71	13.66
Slights	1.20	1.38	1.22	1.18	1.22	1.23	1.34	1.32	1.30	1.26	1.30
Ylights	0.47	0.59	0.55	0.46	0.46	0.45	0.26	0.24	0.23	0.23	0.20
SC-10	0.55	0.54	0.54	0.53	0.53	0.54	0.29	0.27	0.05	0.19	0.31
YC-10	0.22	0.23	0.24	0.20	0.20	0.20	0.06	0.05	0.01	0.04	0.05
Sdi-isopropylated	9.36	9.37	10.50	10.37	8.84	9.35	4.45	4.30	3.97	4.05	3.34
Ydi-isopropylated	3.69	3.99	4.73	4.01	3.31	3.39	0.86	0.78	0.70	0.73	0.52
Sheavies	0.62	0.67	0.72	0.65	0.59	0.79	0.48	0.52	0.45	0.64	0.19
Yheavies	0.25	0.29	0.33	0.25	0.22	0.29	0.09	0.09	0.08	0.12	0.03
Sether	0.40	0.38	0.39	0.41	0.41	0.43	1.26	1.59	1.35	1.37	1.85
Yether	0.16	0.16	0.17	0.16	0.15	0.16	0.24	0.29	0.24	0.25	0.29

Table E.9: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-44	WC-45	WC-46	WC-47	WC-48	WC-49	WC-50	WC-51	WC-52	WC-53	WC-54	WC-55
Time on Stream	201:01:37	202:01:37	203:01:37	204:01:37	206:01:37	207:01:37	207:31:37	208:01:37	208:31:12	217:01:12	218:01:12	219:01:12
Entry Temperature	88	89	89	88	84	83	83	83	83	90	91	91
Temperature	275	275	275	275	274	274	275	275	275	275	275	274
WHSV	1.81	181	1.81	1.81	3.63	3.63	3.63	3.63	3.63	1.28	1.28	1.28
Pump Rate (ml/min)	0.227	0.227	0.227	0.227	0.454	0.454	0.454	0.454	0.454	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	12.90	12.14	11.78	11.65	7.75	7.52	7.79	7.13	7.59	11.50	11.56	12.10
Thymol Selectivity	51.43	50.96	49.51	49.67	36.55	33.74	34.50	33.18	35.30	39.60	39.39	39.85
Thymol Yield	6.63	6.19	5.83	5.78	2.83	2.54	2.69	2.37	2.68	4.55	4.55	4.82
S3-isopropyl-5-methylphenol	**1.65**	**1.55**	**1.51**	**1.38**	**1.08**	**0.77**	**0.76**	**0.67**	**0.79**	**0.78**	**0.89**	**0.89**
Y3-methyl-5-isopropylphenol	0.21	0.19	0.18	0.16	0.08	0.06	0.06	0.05	0.06	0.09	0.10	0.11
S4-isopropyl-3-methylphenol	**10.52**	**10.34**	**9.47**	**9.71**	**8.09**	**6.28**	**6.07**	**5.37**	**5.85**	**6.19**	**6.51**	**6.47**
Y3-methyl-4-isopropylphenol	1.36	1.25	1.11	1.13	0.63	0.47	0.47	0.38	0.44	0.71	0.75	0.78
S2-isopropyl-3-methylphenol	**22.06**	**22.42**	**22.81**	**23.57**	**22.03**	**21.57**	**22.47**	**22.06**	**23.53**	**23.76**	**23.50**	**23.47**
Y3-methyl-2-isopropylphenol	2.84	2.72	2.69	2.74	1.71	1.62	1.75	1.57	1.78	2.73	2.72	2.84
Thymol	60.05	59.77	59.44	58.90	53.95	54.11	54.08	54.14	53.92	56.31	56.03	56.38
3-methyl-5-isopropylphenol	1.93	1.82	1.81	1.64	1.59	1.24	1.19	1.09	1.21	1.11	1.27	1.27
3-methyl-2-isopropylphenol	12.28	12.12	11.36	11.52	11.94	10.07	9.52	8.77	8.93	8.80	9.26	9.15
3-methyl-4-isopropylphenol	25.75	26.29	27.39	27.95	32.52	34.59	35.21	36.00	35.94	33.78	33.43	33.20
STotal.Isomer	**85.65**	**85.27**	**83.30**	**84.33**	**67.75**	**62.35**	**63.80**	**61.28**	**65.46**	**70.33**	**70.30**	**70.69**
YTotal.Isomer	11.05	10.35	9.81	9.82	5.25	4.69	4.97	4.37	4.97	8.09	8.13	8.55
Slights	1.34	1.49	1.34	1.73	1.79	2.04	1.79	1.74	2.09	1.58	1.53	1.67
Ylights	0.17	0.18	0.16	0.20	0.14	0.15	0.14	0.12	0.16	0.18	0.18	0.20
SC-10	0.18	0.17	0.15	0.16	-	-	-	-	-	-	-	-
YC-10	0.02	0.02	0.02	0.02	-	-	-	-	-	-	-	-
Sdi-isopropylated	2.94	2.71	2.69	2.32	1.57	1.25	1.29	1.21	1.07	1.84	1.87	2.06
Ydi-isopropylated	0.38	0.33	0.32	0.27	0.12	0.09	0.10	0.09	0.08	0.21	0.22	0.25
Sheavies	0.73	0.60	1.17	0.44	0.99	1.42	1.54	1.72	1.69	0.94	1.43	1.17
Yheavies	0.09	0.07	0.14	0.05	0.08	0.11	0.12	0.12	0.13	0.11	0.17	0.14
Sether	2.83	3.21	4.55	4.37	19.04	23.81	22.63	24.41	20.53	18.32	18.42	18.26
Yether	0.37	0.39	0.54	0.51	1.47	1.79	1.76	1.74	1.56	2.11	2.13	2.21

Table E.10: Conversion, selectivity and yield data for H-MFI-90 powder

	PW-1	PW-2	PW-3	PW-4	PW-6	PW-9	PW-12	PW-17	PW-19	PW-23	PW-25	PW-29	PW-32
Time on Stream	1:02:06	2:01:00	3:01:00	4:01:00	7:01:00	15:01:00	25:01:00	35:01:00	46:01:00	59:37:00	71:01:00	79:01:00	89:45:00
Entry Temperature	103	103	96	88	90	90	88	86	92	87	86	86	86
Temperature	274	276	276	276	277	275	275	275	275	275	275	275	274
$WHSV_{Wet}$	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guage Pressure (bar)	2	2	2	2	2	3	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3		3	3	3	3	3	3	3
Conversion	27.88	32.13	38.94	51.34	45.59	42.07	32.93	25.43	25.08	19.01	17.34	16.20	16.54
Thymol Selectivity	24.11	41.77	50.94	43.64	58.21	55.02	59.40	59.53	59.09	58.77	58.06	58.28	58.18
Thymol Yield	6.72	13.42	19.84	22.40	26.54	23.15	19.56	15.14	14.82	11.17	10.07	9.44	9.62
S3-isopropyl-5-methylphenol	**6.04**	**5.14**	**4.46**	**3.41**	**4.12**	**5.00**	**3.14**	**2.98**	**2.84**	**2.67**	**2.58**	**2.59**	**2.57**
Y3-methyl-5-isopropylphenol	1.68	1.65	1.74	1.75	1.88	2.10	1.04	0.76	0.71	0.51	0.45	0.42	0.42
S4-isopropyl-3-methylphenol	**5.41**	**9.61**	**11.64**	**10.42**	**15.15**	**13.31**	**18.04**	**18.11**	**18.19**	**17.06**	**16.98**	**16.78**	**16.98**
Y3-methyl-4-isopropylphenol	1.51	3.09	4.53	5.35	6.91	5.60	5.94	4.61	4.56	3.24	2.94	2.72	2.81
S2-isopropyl-3-methylphenol	**0.63**	**1.46**	**2.29**	**2.04**	**3.04**	**2.31**	**5.89**	**6.78**	**7.09**	**7.86**	**8.20**	**8.38**	**8.45**
Y3-methyl-2-isopropylphenol	0.18	0.47	0.89	1.05	1.39	0.97	1.94	1.72	1.78	1.49	1.42	1.36	1.40
Thymol	66.62	72.06	73.47	73.32	72.29	72.75	68.69	68.11	67.76	68.04	67.66	67.74	67.51
3-methyl-5-isopropylphenol	16.69	8.86	6.43	5.73	5.11	6.61	3.64	3.41	3.25	3.10	3.00	3.01	2.98
3-methyl-2-isopropylphenol	14.96	16.57	16.79	17.51	18.81	17.59	20.86	20.73	20.86	19.76	19.78	19.50	19.70
3-methyl-4-isopropylphenol	1.74	2.51	3.31	3.43	3.78	3.05	6.81	7.75	8.13	9.10	9.56	9.75	9.81
STotal.Isomer	**36.19**	**57.97**	**69.33**	**59.52**	**80.52**	**75.64**	**86.47**	**87.40**	**87.20**	**86.37**	**85.82**	**86.04**	**86.18**
YTotal.Isomer	10.09	18.63	27.00	30.55	36.71	31.82	28.48	22.23	21.87	16.42	14.88	13.94	14.25
Slights	6.39	2.36	2.01	1.13	1.19	1.46	0.97	1.02	1.09	1.14	1.21	1.15	1.17
Ylights	1.78	0.76	0.78	0.58	0.54	0.62	0.32	0.26	0.27	0.22	0.21	0.19	0.19
SC-10	19.49	16.46	12.28	7.73	8.18	9.38	5.02	4.64	4.31	4.34	4.11	4.09	4.06
YC-10	5.43	5.29	4.78	3.97	3.73	3.95	1.65	1.18	1.08	0.83	0.71	0.66	0.67
Sdi-isopropylated	7.44	6.59	5.47	4.14	4.31	5.04	2.65	2.03	2.07	1.70	1.62	1.52	1.54
Ydi-isopropylated	2.08	2.12	2.13	2.13	1.96	2.12	0.87	0.52	0.52	0.32	0.28	0.25	0.26
Sheavies	13.24	10.73	7.01	25.91	3.20	5.56	1.39	0.76	0.86	0.75	0.99	0.65	0.55
Yheavies	3.69	3.45	2.73	13.30	1.46	2.34	0.46	0.19	0.22	0.14	0.17	0.11	0.09
Sether	0.92	0.20	0.34	0.23	0.15	0.23	0.65	1.01	1.04	1.51	1.73	1.83	1.86
Yether	0.26	0.06	0.13	0.12	0.07	0.10	0.21	0.26	0.26	0.29	0.30	0.30	0.31

Table E.11: Conversion, selectivity and yield data for H-MFI-90 powder

	PW-35	PW-36	PW-37	PW-38	PW2-40	PW-41	PW-42	PW-43	PW-44	PW-45	PW-46
Time on Stream	92:01:00	93:01:00	94:01:00	95:01:00	97:01:00	98:01:00	103:01:00	103:31:00	104:01:00	104:31:00	105:01:00
Entry Temperature	88	88	88	88	88	88	83	83	84	84	84
Temperature	275	275	275	275	275	274	275	274	274	275	275
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	1.81	1.81	1.81	1.81	1.81
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.302	0.302	0.302	0.302	0.302
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3
Conversion	15.08	14.59	14.06	13.87	13.98	13.74	7.11	6.64	6.68	6.43	6.36
Thymol Selectivity	57.38	57.34	57.02	57.16	56.92	57.24	50.42	49.78	49.93	49.79	49.88
Thymol Yield	8.65	8.36	8.02	7.93	7.96	7.87	3.58	3.30	3.34	3.20	3.17
S3-isopropyl-5-methylphenol	**2.55**	**2.52**	**2.51**	**2.53**	**2.54**	**2.54**	**2.23**	**2.24**	**2.23**	**2.22**	**2.21**
Y3-methyl-5-isopropylphenol	0.38	0.37	0.35	0.35	0.36	0.35	0.16	0.15	0.15	0.14	0.14
S4-isopropyl-3-methylphenol	**16.70**	**16.72**	**16.30**	**16.61**	**16.50**	**16.31**	**15.34**	**15.22**	**15.56**	**15.38**	**15.40**
Y3-methyl-4-isopropylphenol	2.52	2.44	2.29	2.30	2.31	2.24	1.09	1.01	1.04	0.99	0.98
S2-isopropyl-3-methylphenol	**8.95**	**8.86**	**8.97**	**8.90**	**8.89**	**8.99**	**9.49**	**9.50**	**9.58**	**9.44**	**9.51**
Y3-methyl-2-isopropylphenol	1.35	1.29	1.26	1.23	1.24	1.24	0.67	0.63	0.64	0.61	0.60
Thymol	67.05	67.12	67.25	67.09	67.08	67.28	65.08	64.87	64.59	64.81	64.78
3-methyl-5-isopropylphenol	2.97	2.95	2.95	2.97	2.99	2.99	2.88	2.92	2.89	2.89	2.88
3-methyl-2-isopropylphenol	19.51	19.57	19.22	19.49	19.44	19.17	19.80	19.83	20.13	20.01	19.99
3-methyl-4-isopropylphenol	10.46	10.37	10.58	10.45	10.48	10.57	12.25	12.38	12.39	12.29	12.35
STotal.Isomer	**85.57**	**85.43**	**84.80**	**85.21**	**84.85**	**85.08**	**77.48**	**76.74**	**77.30**	**76.82**	**77.00**
YTotal.Isomer	12.90	12.46	11.93	11.82	11.86	11.69	5.51	5.09	5.17	4.94	4.90
Slights	1.02	1.18	1.21	1.15	1.32	1.21	1.58	1.61	1.47	1.64	1.65
Ylights	0.15	0.17	0.17	0.16	0.18	0.17	0.11	0.11	0.10	0.11	0.10
SC-10	3.88	3.86	3.85	3.85	3.86	3.82	3.15	3.13	3.08	3.09	3.09
YC-10	0.58	0.56	0.54	0.53	0.54	0.52	0.22	0.21	0.21	0.20	0.20
Sdi-isopropylated	1.49	1.42	1.43	1.41	1.40	1.38	0.77	0.87	0.91	0.80	0.82
Ydi-isopropylated	0.22	0.21	0.20	0.20	0.20	0.19	0.05	0.06	0.06	0.05	0.05
Sheavies	0.69	0.66	0.87	0.64	0.80	0.54	1.81	1.65	1.07	1.17	0.72
Yheavies	0.10	0.10	0.12	0.09	0.11	0.07	0.13	0.11	0.07	0.07	0.05
Sether	2.33	2.26	2.44	2.33	2.37	2.50	5.34	5.42	5.74	5.66	5.78
Yether	0.35	0.33	0.34	0.32	0.33	0.34	0.38	0.36	0.38	0.36	0.37

Table E.12: Conversion, selectivity and yield data for H-MFI-90 powder (cont.)

	PW-47	PW-48	PW-49	PW-50	PW-51	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59
Time on Stream	116:31:00	117:01:00	117:31:00	118:01:00	127:01:00	135:01:00	137:01:00	139:01:00	141:01:00	141:31:00	180:53:22	188:56:55	190:00:55
Entry Temperature	87	85	85	85	88	86	86	86	86	86	86	89	90
Temperature	274	274	275	275	275	275	274	275	275	275	275	276	276
WHSV	3.62	3.62	3.62	3.62	3.62	0.3	0.3	0.3	0.3	0.3	0.96	0.96	0.96
Pump Rate (ml/min)	0.6042	0.604	0.604	0.604	0.604	0.05	0.05	0.05	0.05	0.05	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	2.00	1.88	1.83	1.71	1.98	26.62	26.28	24.58	27.10	26.94	12.15	11.04	9.31
Thymol Selectivity	23.39	20.73	19.40	17.72	21.73	63.44	62.43	62.69	62.01	62.65	56.25	56.25	56.57
Thymol Yield	0.47	0.39	0.35	0.30	0.43	16.89	16.40	15.41	16.80	16.88	6.83	6.21	5.27
S3-isopropyl-5-methylphenol	**1.23**	**1.00**	**1.02**	**0.90**	**1.13**	**2.86**	**2.92**	**2.99**	**3.00**	**2.81**	**2.61**	**2.43**	**2.30**
Y3-methyl-5-isopropylphenol	0.02	0.02	0.02	0.02	0.02	0.76	0.77	0.74	0.81	0.76	0.32	0.27	0.21
S4-isopropyl-3-methylphenol	**8.46**	**7.36**	**6.65**	**6.16**	**6.75**	**13.40**	**13.81**	**13.71**	**13.82**	**13.96**	**15.40**	**14.97**	**14.53**
Y3-methyl-4-isopropylphenol	0.17	0.14	0.12	0.11	0.13	3.57	3.63	3.37	3.75	3.76	1.87	1.65	1.35
S2-isopropyl-3-methylphenol	**5.55**	**5.24**	**4.80**	**4.84**	**5.77**	**6.74**	**6.79**	**6.45**	**6.69**	**6.78**	**9.10**	**9.70**	**9.49**
Y3-methyl-2-isopropylphenol	0.11	0.10	0.09	0.08	0.11	1.80	1.79	1.58	1.81	1.83	1.10	1.07	0.88
Thymol	60.56	60.38	60.87	59.83	61.42	73.40	72.63	73.03	72.50	72.68	67.48	67.48	68.25
3-methyl-5-isopropylphenol	3.18	2.92	3.19	3.03	3.20	3.31	3.40	3.49	3.51	3.26	3.13	2.92	2.78
3-methyl-2-isopropylphenol	21.90	21.44	20.87	20.81	19.08	15.50	16.07	15.97	16.16	16.20	18.48	17.96	17.53
3-methyl-4-isopropylphenol	14.36	15.26	15.07	16.33	16.30	7.80	7.90	7.51	7.83	7.87	10.91	11.64	11.45
STotal.Isomer	**38.63**	**34.33**	**31.87**	**29.62**	**35.38**	**86.44**	**85.96**	**85.84**	**85.52**	**86.21**	**83.36**	**83.37**	**82.90**
YTotal.Isomer	0.77	0.64	0.58	0.51	0.70	23.01	22.59	21.10	23.17	23.23	10.13	9.20	7.72
Slights	4.25	4.17	4.95	4.88	4.13	1.09	1.20	1.19	1.18	1.21	1.44	1.34	1.05
Ylights	0.08	0.08	0.09	0.08	0.08	0.29	0.32	0.29	0.32	0.33	0.18	0.15	0.10
SC-10	1.08	0.92	0.65	0.51	1.28	4.84	4.85	4.94	4.90	4.77	4.14	3.99	3.94
YC-10	0.02	0.02	0.01	0.01	0.03	1.29	1.27	1.21	1.33	1.28	0.50	0.44	0.37
Sdi-isopropylated	0.17	0.29	0.39	0.39	0.45	2.46	2.61	2.77	2.87	2.56	1.79	1.38	1.17
Ydi-isopropylated	0.00	0.01	0.01	0.01	0.01	0.65	0.69	0.68	0.78	0.69	0.22	0.15	0.11
Sheavies	1.57	3.66	4.18	5.05	8.02	0.82	1.03	0.78	1.21	1.05	0.82	0.85	0.63
Yheavies	0.03	0.07	0.08	0.09	0.16	0.22	0.27	0.19	0.33	0.28	0.10	0.09	0.06
Sether	20.22	20.66	20.73	19.25	16.39	0.76	0.75	0.74	0.73	0.71	2.26	2.45	2.57
Yether	0.40	0.39	0.38	0.33	0.32	0.20	0.20	0.18	0.20	0.19	0.27	0.27	0.24

Table E.13: Conversion, selectivity and yield data for microchannel reactor

	MR-1	MR-2	MR-3	MR-4	MR-5	MR-6	MR-7	MR-8	MR-9	MR-10
Time on Stream	2:42:36	42:14:51	59:07:27	65:04:27	75:09:27	88:56:27	99:05:27	113:01:27	123:12:27	135:38:27
Temperature	275	275	275	276	276	275	275	275	275	276
Entry Temperature	77	75	75	77	77	77	77	77	77	76
WHSV	1.85	1.85	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.001	0.001	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	3	3	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	5.46	3.16	3.65	2.47	1.98	2.54	1.90	2.58	1.99	1.81
Thymol Selectivity	52.80	23.73	22.04	24.57	23.90	30.05	27.47	37.61	32.07	29.33
Thymol Yield	2.88	0.75	0.80	0.61	0.47	0.76	0.52	0.97	0.64	0.53
S3-isopropyl-5-methylphenol	**2.74**	**0.92**	**1.15**	**1.09**	**0.96**	**1.23**	**1.17**	**1.76**	**1.73**	**1.81**
Y3-methyl-5-isopropylphenol	0.15	0.03	0.04	0.03	0.02	0.03	0.02	0.05	0.03	0.03
S4-isopropyl-3-methylphenol	**7.15**	**1.20**	**1.17**	**1.42**	**1.43**	**1.87**	**1.86**	**2.96**	**3.07**	**2.77**
Y3-methyl-4-isopropylphenol	0.39	0.04	0.04	0.04	0.03	0.05	0.04	0.08	0.06	0.05
S2-isopropyl-3-methylphenol	**9.13**	**1.62**	**1.30**	**2.07**	**2.60**	**3.82**	**3.79**	**5.10**	**5.33**	**4.96**
Y3-methyl-2-isopropylphenol	0.50	0.05	0.05	0.05	0.05	0.10	0.07	0.13	0.11	0.09
Thymol	73.52	86.37	85.90	84.28	82.76	81.27	80.10	79.30	76.00	75.45
3-methyl-5-isopropylphenol	3.82	3.33	4.48	3.74	3.31	3.33	3.42	3.70	4.10	4.66
3-methyl-2-isopropylphenol	9.96	4.38	4.55	4.86	4.95	5.07	5.43	6.24	7.27	7.12
3-methyl-4-isopropylphenol	12.71	5.91	5.06	7.11	8.99	10.33	11.05	10.75	12.63	12.76
STotal.Isomer	**71.82**	**27.47**	**25.65**	**29.15**	**28.88**	**36.97**	**34.30**	**47.42**	**42.20**	**38.87**
YTotal.Isomer	3.92	0.87	0.94	0.72	0.57	0.94	0.65	1.22	0.84	0.71
Slights	2.70	6.00	4.78	5.10	4.62	4.03	4.66	4.35	4.18	5.07
Ylights	0.15	0.19	0.17	0.13	0.09	0.10	0.09	0.11	0.08	0.09
SC-10	3.43	17.90	23.66	19.93	15.95	17.24	12.68	11.37	8.16	9.25
YC-10	0.19	0.57	0.86	0.49	0.32	0.44	0.24	0.29	0.16	0.17
Sdi-isopropylated	0.92	1.11	0.97	0.70	0.75	0.62	0.18	-	-	0.19
Ydi-isopropylated	0.05	0.04	0.04	0.02	0.01	0.02	0.00	-	-	0.00
Sheavies	11.24	7.79	7.95	6.77	7.48	7.47	6.71	8.31	8.91	6.53
Yheavies	0.61	0.25	0.29	0.17	0.15	0.19	0.13	0.21	0.18	0.12
Sether	2.90	6.60	0.31	1.03	1.33	1.55	1.92	1.48	2.42	1.85

Table E.14: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-11	MR-12	MR-13	MR-14	MR-15	MR-16	MR-17	MR-18	MR-19	MR-20
Time on Stream	145:14:27	157:10:27	169:09:27	180:42:28	191:59:37	204:16:37	216:04:37	228:08:37	261:10:37	271:52:37
Temperature	300	300	300	300	300	300	300	300	325	325
Entry Temperature	76	74	70	74	73	73	73	74	74	73
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	2.74	3.81	4.28	4.93	5.37	4.13	3.77	4.80	1.46	1.79
Thymol Selectivity	30.60	34.05	42.55	50.94	52.44	44.42	44.16	48.79	20.45	24.27
Thymol Yield	0.84	1.30	1.82	2.51	2.82	1.84	1.67	2.34	0.30	0.43
S3-isopropyl-5-methylphenol	**1.55**	**1.76**	**2.06**	**2.57**	**2.87**	**2.36**	**4.38**	**6.11**	**1.96**	**2.69**
Y3-methyl-5-isopropylphenol	0.04	0.07	0.09	0.13	0.15	0.10	0.17	0.29	0.03	0.05
S4-isopropyl-3-methylphenol	**2.45**	**2.90**	**4.54**	**5.93**	**6.19**	**9.46**	**5.20**	**5.77**	**2.69**	**3.21**
Y3-methyl-4-isopropylphenol	0.07	0.11	0.19	0.29	0.33	0.39	0.20	0.28	0.04	0.06
S2-isopropyl-3-methylphenol	**3.91**	**4.19**	**8.78**	**10.75**	**12.28**	**11.81**	**9.06**	**6.75**	**5.40**	**5.45**
Y3-methyl-2-isopropylphenol	0.11	0.16	0.38	0.53	0.66	0.49	0.34	0.32	0.08	0.10
Thymol	79.47	79.35	73.46	72.56	71.08	65.28	70.33	72.36	67.07	68.14
3-methyl-5-isopropylphenol	4.03	4.11	3.55	3.67	3.89	3.46	6.98	9.07	6.41	7.55
3-methyl-2-isopropylphenol	6.37	6.77	7.84	8.45	8.39	13.90	8.28	8.56	8.81	9.00
3-methyl-4-isopropylphenol	10.14	9.77	15.15	15.32	16.64	17.36	14.42	10.02	17.71	15.30
STotal.Isomer	**38.50**	**42.91**	**57.93**	**70.20**	**73.77**	**68.05**	**62.80**	**67.42**	**30.49**	**35.62**
YTotal.Isomer	1.05	1.64	2.48	3.46	3.96	2.81	2.37	3.24	0.44	0.64
Slights	3.80	3.62	2.95	2.27	2.27	2.53	2.99	3.40	5.46	4.55
Ylights	0.10	0.14	0.13	0.11	0.12	0.10	0.11	0.16	0.08	0.08
SC-10	19.75	22.13	9.31	4.67	2.64	1.83	3.33	4.94	2.47	3.63
YC-10	0.54	0.84	0.40	0.23	0.14	0.08	0.13	0.24	0.04	0.06
Sdi-isopropylated	0.54	0.58	0.30	0.56	0.96	0.58	0.42	0.28	-	-
Ydi-isopropylated	0.01	0.02	0.01	0.03	0.05	0.02	0.02	0.01	-	-
Sheavies	6.31	7.71	13.08	10.47	10.24	14.14	11.04	10.36	7.80	14.49
Yheavies	0.17	0.29	0.56	0.52	0.55	0.58	0.42	0.50	0.11	0.26
Sether	1.39	1.19	2.97	3.10	3.70	5.98	6.31	3.67	6.20	3.81

Table E.15: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-21	MR-22	MR-23	MR-24	MR-25	MR-26	MR-27	MR-28	MR-29	MR-30
Time on Stream	281:34:37	309:39:37	319:52:37	342:40:37	353:19:37	364:28:37	375:51:37	388:30:37	442:02:37	449:27:37
Temperature	325	325	325	325	325	325	325	325	325	325
Entry Temperature	64	74	73	77	77	77	78	77	77	77
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	1.58	1.38	1.42	1.72	1.15	1.04	0.98	1.04	1.00	1.06
Thymol Selectivity	22.30	19.41	15.01	27.88	17.06	12.43	7.41	13.15	10.50	14.04
Thymol Yield	0.35	0.27	0.21	0.48	0.20	0.13	0.07	0.14	0.11	0.15
S3-isopropyl-5-methylphenol	**2.31**	**2.29**	**1.78**	**5.89**	**3.83**	**2.39**	**1.05**	**0.78**	**0.47**	**0.98**
Y3-methyl-5-isopropylphenol	0.04	0.03	0.03	0.10	0.04	0.02	0.01	0.01	0.00	0.01
S4-isopropyl-3-methylphenol	**3.33**	**3.13**	**2.71**	**3.73**	**2.56**	**1.77**	**0.85**	**1.94**	**1.47**	**2.24**
Y3-methyl-4-isopropylphenol	0.05	0.04	0.04	0.06	0.03	0.02	0.01	0.02	0.01	0.02
S2-isopropyl-3-methylphenol	**5.53**	**4.35**	**3.89**	**3.03**	**2.31**	**2.12**	**2.17**	**3.40**	**3.44**	**4.03**
Y3-methyl-2-isopropylphenol	0.09	0.06	0.06	0.05	0.03	0.02	0.02	0.04	0.03	0.04
Thymol	66.64	66.50	64.18	68.78	66.23	66.45	64.53	68.21	66.13	65.97
3-methyl-5-isopropylphenol	6.89	7.86	7.61	14.53	14.88	12.78	9.13	4.07	2.97	4.60
3-methyl-2-isopropylphenol	9.95	10.73	11.58	9.20	9.92	9.45	7.44	10.07	9.25	10.51
3-methyl-4-isopropylphenol	16.52	14.91	16.64	7.48	8.97	11.32	18.90	17.65	21.65	18.92
STotal.Isomer	**33.46**	**29.19**	**23.39**	**40.53**	**25.76**	**18.71**	**11.48**	**19.28**	**15.87**	**21.28**
YTotal.Isomer	0.53	0.40	0.33	0.70	0.30	0.19	0.11	0.20	0.16	0.23
Slights	4.94	5.78	7.21	5.08	6.98	8.01	7.44	7.31	7.73	6.57
Ylights	0.08	0.08	0.10	0.09	0.08	0.08	0.07	0.08	0.08	0.07
SC-10	1.30	0.94	1.33	2.04	2.26	0.89	1.95	0.20	-	-
YC-10	0.02	0.01	0.02	0.04	0.03	0.01	0.02	0.00	-	-
Sdi-isopropylated	-	-	-	-	-	-	-	-	-	-
Ydi-isopropylated	-	-	-	-	-	-	-	-	-	-
Sheavies	12.10	12.53	20.06	14.34	6.63	7.07	7.17	6.72	6.48	7.62
Yheavies	0.19	0.17	0.28	0.25	0.08	0.07	0.07	0.07	0.06	0.08
Sether	6.40	4.69	3.85	0.92	1.21	1.65	2.12	3.02	3.31	2.97

Table E.16: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-31	MR-32	MR-33	MR-34	MR-35	MR-36	MR-37
Time on Stream	451:02:37	457:30:37	463:20:37	475:24:37	480:11:37	489:30:37	499:54:37
Temperature	275	275	274	275	275	274	275
Entry Temperature	76	74	76	76	77	78	78
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3
Conversion	1.00	1.12	1.68	1.89	1.88	1.97	2.11
Thymol Selectivity	9.54	13.03	25.88	29.59	25.26	24.05	24.40
Thymol Yield	0.10	0.15	0.43	0.56	0.47	0.47	0.51
S3-isopropyl-5-methylphenol	**0.59**	**0.88**	**1.36**	**1.44**	**0.93**	**1.78**	**1.02**
Y3-methyl-5-isopropylphenol	0.01	0.01	0.02	0.03	0.02	0.04	0.02
S4-isopropyl-3-methylphenol	**1.49**	**2.19**	**3.56**	**4.10**	**3.55**	**4.17**	**3.93**
Y3-methyl-4-isopropylphenol	0.01	0.02	0.06	0.08	0.07	0.08	0.08
S2-isopropyl-3-methylphenol	**2.94**	**4.47**	**8.50**	**9.68**	**10.05**	**8.85**	**10.40**
Y3-methyl-2-isopropylphenol	0.03	0.05	0.14	0.18	0.19	0.17	0.22
Thymol	65.52	63.34	65.85	66.03	63.49	61.89	61.39
3-methyl-5-isopropylphenol	4.04	4.29	3.45	3.22	2.33	4.59	2.56
3-methyl-2-isopropylphenol	10.24	10.62	9.07	9.15	8.93	10.74	9.89
3-methyl-4-isopropylphenol	20.19	21.74	21.64	21.60	25.25	22.78	26.16
STotal.Isomer	**14.55**	**20.58**	**39.31**	**44.82**	**39.79**	**38.86**	**39.74**
YTotal.Isomer	0.15	0.23	0.66	0.85	0.75	0.77	0.84
Slights	7.00	6.79	4.68	4.40	3.50	4.06	4.17
Ylights	0.07	0.08	0.08	0.08	0.07	0.08	0.09
SC-10	-	-	0.43	0.35	0.32	0.73	-
YC-10	-	-	0.01	0.01	0.01	0.01	-
Sdi-isopropylated	-	-	-	0.36	0.49	0.20	0.36
Ydi-isopropylated	-	-	-	0.01	0.01	0.00	0.01
Sheavies	8.75	7.31	10.50	8.76	7.94	11.51	11.53
Yheavies	0.09	0.08	0.18	0.17	0.15	0.23	0.24
Sether	3.29	4.87	7.76	9.83	15.82	14.14	16.12

Table E.17: Conversion, selectivity and yield data for H-MFI-90 powder repeat

	PW-1	PW-3	PW-5	PW-7	PW-11	PW-15	PW-20	PW-23	PW-28	PW-29
Time on Stream	07:52:00	08:58:06	11:00:07	13:04:06	20:02:06	31:58:07	38:00:07	41:00:06	46:56:06	55:00:00
Entry Temperature	90	91	91	93	92	92	92	92	91	92
Temperature	275	275	275	274	275	274	275	274	275	275
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	25.06	36.71	38.17	37.28	33.07	30.88	25.07	24.06	24.86	25.22
Thymol Selectivity	26.15	59.45	60.36	61.20	61.88	61.84	62.63	62.52	61.69	61.70
Thymol Yield	6.55	21.83	23.04	22.82	20.46	19.10	15.70	15.04	15.34	15.56
S3-isopropyl-5-methylphenol	**7.52**	**3.97**	**3.82**	**3.68**	**3.34**	**3.20**	**2.93**	**2.91**	**2.88**	**2.77**
Y3-methyl-5-isopropylphenol	1.88	1.46	1.46	1.37	1.10	0.99	0.73	0.70	0.72	0.70
S4-isopropyl-3-methylphenol	**6.89**	**15.15**	**15.76**	**16.06**	**16.42**	**16.71**	**16.05**	**15.93**	**16.82**	**16.44**
Y3-methyl-4-isopropylphenol	1.73	5.56	6.01	5.99	5.43	5.16	4.02	3.83	4.18	4.15
S2-isopropyl-3-methylphenol	**0.70**	**3.18**	**3.42**	**3.73**	**4.24**	**4.59**	**5.09**	**5.26**	**5.83**	**5.89**
Y3-methyl-2-isopropylphenol	0.18	1.17	1.30	1.39	1.40	1.42	1.28	1.26	1.45	1.49
Thymol	63.37	72.73	72.41	72.27	72.05	71.62	72.24	72.18	70.73	71.09
3-methyl-5-isopropylphenol	18.22	4.85	4.59	4.35	3.89	3.71	3.37	3.36	3.30	3.19
3-methyl-2-isopropylphenol	16.70	18.53	18.90	18.97	19.12	19.36	18.51	18.39	19.29	18.94
3-methyl-4-isopropylphenol	1.71	3.89	4.10	4.41	4.94	5.32	5.87	6.07	6.68	6.79
STotal.Isomer	**41.27**	**81.74**	**83.36**	**84.68**	**85.88**	**86.35**	**86.70**	**86.62**	**87.23**	**86.80**
YTotal.Isomer	10.34	30.01	31.82	31.57	28.40	26.66	21.73	20.84	21.69	21.89
Slights	3.69	1.11	1.02	0.94	0.96	0.93	0.96	0.97	0.95	1.07
Ylights	0.92	0.41	0.39	0.35	0.32	0.29	0.24	0.23	0.24	0.27
SC-10	19.53	8.95	8.19	7.57	6.79	6.50	6.06	6.06	5.32	5.36
YC-10	4.89	3.29	3.13	2.82	2.24	2.01	1.52	1.46	1.32	1.35
Sdi-isopropylated	6.15	3.25	3.05	2.84	2.28	2.09	1.64	1.62	1.76	1.86
Ydi-isopropylated	1.54	1.19	1.16	1.06	0.75	0.64	0.41	0.39	0.44	0.47
Sheavies	8.17	2.06	1.60	1.32	1.10	1.03	0.81	0.86	0.77	0.76
Yheavies	2.05	0.75	0.61	0.49	0.36	0.32	0.20	0.21	0.19	0.19
Sether	0.64	0.12	0.13	0.21	0.37	0.41	0.53	0.59	0.72	0.88
Yether	0.16	0.05	0.05	0.08	0.12	0.13	0.13	0.14	0.18	0.22

Table E.18: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-35	PW-37	PW-39	PW-43	PW-46	PW-47	PW-48	PW-49	PW-50	PW-51
Time on Stream	60:00:07	68:00:07	81:00:06	89:00:06	93:50:06	103:44:21	104:00:21	105:00:21	106:00:21	107:00:21
Entry Temperature	93	86	93	94	94	92	92	92	92	93
Temperature	274	275	276	275	275	275	274	275	275	274
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	20.90	20.08	17.84	16.40	15.83	15.10	15.45	15.77	15.28	14.40
Thymol Selectivity	61.07	61.02	60.74	60.86	61.29	60.48	59.29	59.16	59.17	58.73
Thymol Yield	12.77	12.26	10.83	9.98	9.70	9.13	9.16	9.33	9.04	8.46
S3-isopropyl-5-methylphenol	**2.73**	**2.68**	**2.60**	**2.54**	**2.52**	**2.43**	**2.51**	**2.57**	**2.45**	**2.47**
Y3-methyl-5-isopropylphenol	0.57	0.54	0.46	0.42	0.40	0.37	0.39	0.41	0.37	0.36
S4-isopropyl-3-methylphenol	**16.55**	**16.07**	**15.95**	**15.43**	**15.16**	**14.61**	**15.49**	**16.04**	**15.55**	**15.35**
Y3-methyl-4-isopropylphenol	3.46	3.23	2.84	2.53	2.40	2.21	2.39	2.53	2.38	2.21
S2-isopropyl-3-methylphenol	**6.61**	**6.75**	**6.88**	**7.10**	**7.12**	**7.65**	**7.95**	**7.86**	**8.05**	**8.16**
Y3-methyl-2-isopropylphenol	1.38	1.36	1.23	1.16	1.13	1.16	1.23	1.24	1.23	1.18
Thymol	70.23	70.52	70.49	70.83	71.19	71.01	69.55	69.08	69.42	69.33
3-methyl-5-isopropylphenol	3.14	3.10	3.02	2.95	2.92	2.85	2.95	3.01	2.88	2.91
3-methyl-2-isopropylphenol	19.04	18.57	18.50	17.95	17.61	17.16	18.17	18.73	18.25	18.12
3-methyl-4-isopropylphenol	7.60	7.81	7.99	8.26	8.27	8.98	9.33	9.18	9.45	9.64
STotal.Isomer	**86.96**	**86.53**	**86.18**	**85.92**	**86.09**	**85.18**	**85.25**	**85.64**	**85.22**	**84.70**
YTotal.Isomer	18.18	17.38	15.37	14.09	13.63	12.86	13.17	13.50	13.03	12.20
Slights	1.05	1.03	1.08	1.07	0.99	1.10	1.03	1.08	1.08	1.14
Ylights	0.22	0.21	0.19	0.17	0.16	0.17	0.16	0.17	0.17	0.16
SC-10	4.97	4.99	5.13	4.60	4.94	4.93	4.43	4.41	4.29	4.29
YC-10	1.04	1.00	0.91	0.75	0.78	0.74	0.68	0.69	0.66	0.62
Sdi-isopropylated	1.61	1.61	1.42	1.32	1.09	1.22	1.37	1.41	1.41	1.36
Ydi-isopropylated	0.34	0.32	0.25	0.22	0.17	0.18	0.21	0.22	0.22	0.20
Sheavies	0.65	0.80	0.66	1.03	0.66	0.78	0.83	0.72	0.74	0.79
Yheavies	0.14	0.16	0.12	0.17	0.10	0.12	0.13	0.11	0.11	0.11
Sether	1.05	1.17	1.29	1.46	1.50	1.84	2.20	1.94	2.30	2.51
Yether	0.22	0.23	0.23	0.24	0.24	0.28	0.34	0.31	0.35	0.36

Table E.19: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59	PW-60	PW-61	PW-62	PW-63	PW-64	PW-65	PW-66
Time on Stream	132:00:55	133:00:55	134:00:55	135:00:55	135:54:55	152:00:55	163:14:55	179:00:55	181:00:55	182:48:55	188:00:55	188:56:55	190:00:55	191:00:55	198:04:55
Entry Temperature	92	91	92	93	94	94	96	95	95	95	89	89	90	89	90
Temperature	276	275	275	275	275	275	274	275	274	274	275	276	276	275	276
WHSV	0.72	0.72	0.72	0.72	0.72	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (m/min)	0.12	0.12	0.12	0.12	0.12	0.05	0.05	0.05	0.05	0.05	0.2	0.2	0.2	0.2	0.2
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	15.07	15.10	14.89	14.88	13.40	27.97	28.71	27.09	26.82	27.20	7.94	7.57	6.92	6.59	5.03
Thymol Selectivity	58.98	58.49	59.56	58.44	58.75	63.17	61.47	62.94	62.84	62.46	52.94	52.78	52.07	50.10	49.89
Thymol Yield	8.89	8.83	8.87	8.70	7.87	17.67	17.65	17.05	16.85	16.99	4.20	3.99	3.60	3.30	2.51
S3-isopropyl-5-methylphenol	**2.61**	**2.57**	**2.45**	**2.52**	**2.42**	**2.91**	**2.72**	**2.63**	**2.78**	**2.82**	**2.28**	**2.34**	**2.28**	**2.19**	**2.18**
Y3-methyl-5-isopropylphenol	0.39	0.39	0.36	0.38	0.32	0.81	0.78	0.71	0.75	0.77	0.18	0.18	0.16	0.14	0.11
S4-isopropyl-3-methylphenol	**16.03**	**15.84**	**15.14**	**15.76**	**15.51**	**14.26**	**14.49**	**14.44**	**14.43**	**14.76**	**15.32**	**16.26**	**15.16**	**14.51**	**13.80**
Y3-methyl-4-isopropylphenol	2.42	2.39	2.25	2.35	2.08	3.99	4.16	3.91	3.87	4.01	1.22	1.23	1.05	0.96	0.69
S2-isopropyl-3-methylphenol	**8.00**	**8.05**	**8.21**	**8.21**	**8.28**	**6.66**	**6.53**	**6.80**	**6.91**	**6.78**	**9.36**	**9.09**	**9.13**	**8.67**	**8.97**
Y3-methyl-2-isopropylphenol	1.21	1.22	1.22	1.22	1.11	1.86	1.87	1.84	1.85	1.85	0.74	0.69	0.63	0.57	0.45
Thymol	68.88	68.85	69.77	68.81	69.14	72.61	72.14	72.50	72.26	71.94	66.26	65.59	66.21	66.39	66.67
3-methyl-5-isopropylphenol	3.05	3.03	2.87	2.97	2.85	3.35	3.20	3.03	3.20	3.25	2.86	2.91	2.90	2.90	2.92
3-methyl-2-isopropylphenol	18.73	18.65	17.74	18.55	18.26	16.39	17.00	16.63	16.60	17.00	19.18	20.21	19.28	19.23	18.44
3-methyl-4-isopropylphenol	9.34	9.47	9.62	9.67	9.74	7.65	7.66	7.84	7.94	7.81	11.71	11.29	11.61	11.48	11.98
STotal.Isomer	**85.62**	**84.96**	**85.36**	**84.94**	**84.96**	**87.00**	**85.21**	**86.82**	**86.96**	**86.83**	**79.90**	**80.47**	**78.65**	**75.46**	**74.84**
YTotal.Isomer	12.90	12.83	12.71	12.64	11.38	24.34	24.46	23.52	23.32	23.62	6.34	6.09	5.44	4.97	3.76
Slights	1.32	1.40	1.04	1.18	1.05	0.97	1.51	1.02	1.07	0.92	1.33	0.90	1.42	2.95	1.87
Ylights	0.20	0.21	0.15	0.18	0.14	0.27	0.43	0.28	0.29	0.25	0.11	0.07	0.10	0.19	0.09
SC-10	4.20	4.20	4.25	4.13	3.96	4.97	4.79	4.81	4.76	4.88	3.29	3.37	3.35	3.76	3.12
YC-10	0.63	0.63	0.63	0.62	0.53	1.39	1.38	1.30	1.28	1.33	0.26	0.25	0.23	0.25	0.16
Sdi-isopropylated	1.41	1.50	1.35	1.44	1.32	2.26	2.47	2.22	2.20	2.26	1.00	0.92	0.91	0.79	0.63
Ydi-isopropylated	0.21	0.23	0.20	0.21	0.18	0.63	0.71	0.60	0.59	0.61	0.08	0.07	0.06	0.05	0.03
Sheavies	0.66	0.92	0.85	0.96	0.81	0.72	0.99	0.81	0.73	0.84	0.87	0.72	0.94	0.68	0.81
Yheavies	0.10	0.14	0.13	0.14	0.11	0.20	0.28	0.22	0.20	0.23	0.07	0.05	0.06	0.04	0.04
Sether	1.95	2.10	2.15	2.29	2.36	0.79	0.87	0.86	0.85	0.82	4.83	4.54	4.85	4.94	5.03
Yether	0.29	0.32	0.32	0.34	0.32	0.22	0.25	0.23	0.23	0.22	0.38	0.34	0.34	0.33	0.25

Table E.20: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-67	PW-68	PW-69	PW-70	PW-71	PW-72	PW-73	PW-74	PW-75	PW-76	PW-77	PW-78
Time on Stream	201:00:55	201:30:55	201:58:55	205:00:55	205:30:55	206:00:55	206:30:55	232:10:55	233:30:55	236:32:55	238:30:55	246:36:55
Entry Temperature	90	90	89	85	85	85	85	93	93	92	92	90
Temperature	274	275	275	275	275	275	275	274	275	275	275	275
WHSV	1.81	1.81	1.81	3.62	3.62	3.62	3.62	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.302	0.302	0.302	0.604	0.604	0.604	0.604	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	2.60	2.47	2.42	1.36	0.81	0.92	0.94	1.33	1.41	1.37	1.34	1.25
Thymol Selectivity	34.18	32.36	32.29	3.14	4.53	3.94	3.48	11.19	9.96	10.82	9.89	10.31
Thymol Yield	0.89	0.80	0.78	0.04	0.04	0.04	0.03	0.15	0.14	0.15	0.13	0.13
S3-isopropyl-5-methylphenol	**1.65**	**1.55**	**1.50**	**0.32**	**0.43**	**0.29**	**0.54**	**0.86**	**0.89**	**0.42**	**0.73**	**0.72**
Y3-methyl-5-isopropylphenol	0.04	0.04	0.04	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
S4-isopropyl-3-methylphenol	**9.92**	**9.57**	**9.55**	**1.01**	**1.59**	**1.30**	**1.50**	**3.24**	**2.94**	**2.76**	**2.61**	**3.15**
Y3-methyl-4-isopropylphenol	0.26	0.24	0.23	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04
S2-isopropyl-3-methylphenol	**7.12**	**6.58**	**6.76**	**1.38**	**2.22**	**2.11**	**1.82**	**6.63**	**6.20**	**6.47**	**5.78**	**6.17**
Y3-methyl-2-isopropylphenol	0.18	0.16	0.16	0.02	0.02	0.02	0.02	0.09	0.09	0.09	0.08	0.08
Thymol	64.65	64.65	64.45	53.64	51.65	51.57	47.45	51.02	49.84	52.87	52.03	50.67
3-methyl-5-isopropylphenol	3.11	3.11	3.00	5.45	4.95	3.77	7.30	3.93	4.47	2.03	3.83	3.53
3-methyl-2-isopropylphenol	18.77	19.11	19.06	17.27	18.13	16.98	20.44	14.79	14.70	13.49	13.74	15.47
3-methyl-4-isopropylphenol	13.47	13.14	13.49	23.64	25.27	27.67	24.82	30.26	30.99	31.61	30.41	30.33
STotal.Isomer	**52.86**	**50.06**	**50.11**	**5.85**	**8.77**	**7.63**	**7.33**	**21.93**	**19.99**	**20.46**	**19.02**	**20.36**
YTotal.Isomer	1.37	1.24	1.21	0.08	0.07	0.07	0.07	0.29	0.28	0.28	0.25	0.26
Slights	2.94	3.32	3.26	5.64	9.96	8.37	8.49	5.58	5.49	5.75	5.74	5.82
Ylights	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.07	0.08	0.08	0.08	0.07
SC-10	1.65	1.54	1.51	-	-	-	-	-	-	-	-	-
YC-10	0.04	0.04	0.04	-	-	-	-	-	-	-	-	-
Sdi-isopropylated	0.26	0.26	0.20	-	-	-	-	0.29	0.29	0.32	0.33	0.36
Ydi-isopropylated	0.01	0.01	0.00	-	-	-	-	0.00	0.00	0.00	0.00	0.00
Sheavies	1.16	1.35	1.05	4.57	4.29	4.06	4.64	1.99	4.62	2.82	3.13	1.68
Yheavies	0.03	0.03	0.03	0.06	0.03	0.04	0.04	0.03	0.06	0.04	0.04	0.02
Sether	15.08	16.02	15.78	5.36	7.33	6.85	7.25	19.11	22.12	21.19	20.45	17.46
Yether	0.39	0.40	0.38	0.07	0.06	0.06	0.07	0.25	0.31	0.29	0.27	0.22

Appendix

E.

E.2 Experimental data

In this section the conversion, selectivity, and yield of the respective compounds is given at steady state and the first 100 hours where the initial deactivation occurred. The experimental runs conducted in the fixed-bed reactor were for the H-MFI-90 extrudates, H-MFI-90 powder, simulated washcoating and H-MFI-90 powder repeat catalysts, as well as in the microreactor configuration (75% Zeolite washcoating).

Appendix: Simulated washcoating GC product analysis

Table 0.1: GC raw data for H-MFI-90 extrudates

EXTRUDATE		EX-1	EX-2	EX-3	EX-4	EX-5	EX-6	EX-7	EX-8	EX-9	EX-10	EX-11	EX-12	EX-13	EX-14
Time on Stream		1:22:38	2:22:48	7:26:48	9:26:48	11:30:48	13:27:48	18:08:48	30:30:48	37:20:48	57:55:46	67:10:46	77:10:46	80:09:46	83:05:44
Entry Temperature		90	90	91	91	92	93	93	93	92	91	93	93	86	93
Temperature		275	275	275	274	275	274	275	275	275	275	274	275	275	276
WHSV		1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70							5.9	7.6	13.3	19.6	12.5	21.8	36.8	21.7
???	± 5.04	19.7	9	3.7	7.9	7.9	4.4	3.2	1.9	0.5	1	1.4	1.1	1.8	1.6
phenol	± 5.26			2.8	0.9	1.4	1.6	1.4	1.5	2.4	4	2.5	3.9	6.8	4.5
o-Cresol	± 5.35	9.1	35.6	9.2	9.8	1.2	2.3	2.4	2.5	3.3	7.2	3.4	7.4	12.2	6
p-Cresol	± 5.60	205.1	114.9	56.1	56.9	45.4	24.6	23.9	24	35.4	66.6	35.3	61.4	105.1	56.1
m-Cresol	± 5.80	4324.9	5535.5	5003.5	6407	5108.5	2692.9	2823.4	3012.1	4742.6	9491	4997.7	9075.1	15653.8	8364.1
???	± 6.00	6.8	5.6	3.6	4.5	4.4	1.3	2.3	2.4	4	6.8	3.5	7	8.1	5.7
2,4-Xylenol	± 6.20	35.5	29.6	15.9	11.4	7.8	3.3	2.9	2.5	3.1	5.7	2.7	3.7	8	4.5
2,5-Xylenol	± 6.50	11.5	13.4	10.4	11.1	9.1	4.6	3.7	4.1	6	8.6	4.8	9	13.1	7.1
2,3-Xylenol	± 6.74	3.8	15.8	5.7	7	4.7	2.7	2	1.7	3.4	3.8	1.6	4.3	4.5	2.8
???	± 6.90	25.5	24.1	12.4	10.5	2.3	2.7	2.2	2	2.5	2.7	2	2.7	3.8	1.5
???	± 7.03						0.6	0.8		0.6	0.6		0.6		
???	± 7.16	44.5	50.7	25.6	17.8	12.5	4.7	3.7	2.9	3.7	4.6	2	4.2	5.5	2.8
2-Isopropyl-4-methyl Phenol	± 7.30	38.8	52.3	48	56.4	48.7	22.4	22.6	21.1	31.5	46.1	24.2	42.8	72.3	38.8
???	± 7.49	10.7	10.3	5.6	9.2	10.2	3.9	3.2	2.6	3.7	3.7	2.5	3.8	4.9	2.9
Thymol isomer (2,3)	± 7.60	22.6	47.2	95.6	185.3	184.8	95.2	111	125.6	225.2	365	190.3	356.1	640.3	336.7
???	± 7.73	51.4	59.4	37.9	32.9	25.1	11	8.8	7.5	9	12.5	6.2	10	15	7.7
Thymol	± 7.90	84.9	2358.6	4059.6	5883	5120.9	2453.3	2452.1	2334.6	3582.1	5300.6	2605.9	4796.9	7986.7	4175.9
????	± 8.19	63.2	65	41.9	39.7	30.4	13.9	10.7	9.2	13.1	17.8	7.6	145	22.3	12.3
????	± 8.33	252.7	411.4	378.8	376.6	290.7	130.2	109.3	86.9	109	153.1	73.5	120.8	181.4	95.3
6-n-Propyl-3-Methyl Phenol	± 8.40	7.6	12	40.8	90.3	94.7	28.2	56.5	57.4	96.4	116.3	57.4	111.1	179.3	96.3
2,6-Diisoprop.-3-Met. Phen.	± 8.55	108.1	3.6	66.3	53.2	38.5	16.4	13.5	9.6	12.4	15.8	7.4	12.3	17.7	9.3
5,3 Thymol isomer	± 8.67	394.9	855.7	949.3	995.4	790.1	340.9	302	249.4	342.6	436.1	219.9	358.4	561.3	294.5
4,3 Thymol isomer	± 8.78	169.4	472.6	804.7	1146	1024.8	463.9	473.8	443.7	737.4	1059.5	502.2	944	1564.6	819.1
C-13 fraction (13.02)	± 8.83	21.8	14.7	5.9	4	2.6	1.1	1.1	0.7	0.9	1.1	0.8	1.1	3.9	1.1
????	± 9.22	8	160.7	127.8	91.5	60.7	24.1	17.7	12.6	12.6	12.7	8.3	10	13.6	8.8
????	± 9.48	65	92.8	64.9	54.6	42.3	18.4	14.8	11.4	16.4	20.2	8.3	17.1	25.3	10.2
????	± 9.60	23	34.6	19	12.4	7.6	5.3	2.8	2.3	2.9	3.5	2.1	3.4	2.6	4.5
????	± 10.30	143.1	234.7	139.6	77	48.6	18.4	11.6	6.9	9.1	7.5	3.8	6.3	8.1	2.6
????	± 10.70	39.3	49.3	26.7	13.6	10.2	3.7	2.6	2.2	1.6	2.3	2.2	1.3	2.8	2.3
4,6-Diisoprop.-3-Met. Phen.	± 11.18	95.9	340.5	719.6	1009.6	923.7	405.1	400	360.6	547.4	597.6	298.8	526.7	834	447.1
????	± 11.30	9.1	2.1	4.7	1.8	2.8									
????	± 11.80	32.1	40.9	16	4.9	3.4									
????	± 12.09	3.8	18.5												
????	± 12.21	3.2	10.6	19.1	18.7	15.4	6.4	8.5	6.1	9.7	11.6	3.8	9.5	11.2	6.5
5,6-Diisoprop.-3-Met. Phen.	± 12.70	17	50.4	72.3	69.3	45.5	35.3	34.4	29.2	44.1	47.5	23.3	40.1	64.3	32.9
Heavies	± 13.04	37.4	10.2	99.9	49.5	100.5	21.9	13.7	10.5	12.7	15.5	8.2	10.3	16.1	9.2
Heavies		11.7	152.7	106.7	84.8	58.3	47.8	15	12.3	13	13.4	12.3	13.2	15.4	14.3

Table 0.2: GC raw data for H-MFI-90 extrudates (cont.)

EXTRUDATE		EX-15	EX-16	EX-17	EX-18	EX-19	EX-20	EX-21	EX-22	EX-23	EX-24	EX-25	EX-26	EX-27	EX-28	EX-29
Time on Stream		115:13	117:12	119:12	121:13	125:06	144:01	146:23	150:07	159:10	161:09	171:12	172:05	173:19	174:08	174:34
Entry Temperature		94	94	94	94	92	92	93	93	93	92	94	96	96	95	95
Temperature		275	275	275	275	275	275	276	275	275	276	275	274	274	275	275
WHSV		0.6	0.6	0.6	0.6	0.6	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.08	0.08	0.08	0.08	0.08	0.04	0.04	0.04	0.04	0.04	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	18.7	17.3	14.1	12.1	18.4	3.5	5.4	9.4	7	2.8	18.4	15	19.6	20.9	31.4
???	± 5.04	1.7	2.1	1.4	1.7	1.8	0.9	1.8	3.7	3.1	1.8					5.6
phenol	± 5.26	3.4	3.1	2.6	2.6	3.5	1.2	1.3	1.9	1.1		3.5	2.9	3.8	4.1	8.9
o-Cresol	± 5.35	10.7	10.8	6.2	5.2	10.1	4	5.9	13.4	6	2.2	5.2	3.7	5.3	5.8	5.2
p-Cresol	± 5.60	86.2	87.8	52.4	37.8	82.4	33.3	53.5	98.8	52.1	22.4	47.5	37.1	51.3	56.1	81
m-Cresol	± 5.80	11899	12217.1	7221.6	5176.6	11478.3	3877.9	6292	11744.3	6206.2	2585.3	7252	5623	7888.6	8762.6	12787
???	± 6.00	9.2				9.2	2.6	4.4	8.2	4.8	2.5	4.9	4.1	5.6	6.7	16
2,4-Xylenol	± 6.20	9.5	9.8	10.9	3.6	9.2	6.2	10.7	16.6	8.8	3.6	2.4	1.8	2.8	2.2	4
2,5-Xylenol	± 6.50	14.4	13.5	5.2	6.1	12.8	6.7	10.6	19.6	11	2.1	5.1	4.3	5.7	4.2	8
2,3-Xylenol	± 6.74	3.3	2.7	2	1.8	2.8	2.4	2.5	4.4	3.6	1.1	1.5	1.5	1.5	1.2	2.8
???	± 6.90	7.6	5.9	2.6	0.5	4.5	4.8	8.7	10	8.1	2.7	0.5	1.2			
???	± 7.03								4.4							
???	± 7.16	9.8	9.2	5.7	4.2	9.8	6.9	14	21.4	12.7	4.6	2.1	1.6	2.1	2.1	2.1
2-Isopropyl-4-methyl Phenol	± 7.30	78.8	74.7	44.7	35.6	73.3	35	56.6	108.9	57.4	24.5	28.3	21.9	27.8	28.5	41
???	± 7.49	7.3	6.8	4.7	3.6	6.9	4.3	5.8	10.6	11.3	2.5	1.6	1.8	1.6	1.5	1.3
Thymol isomer (2,3)	± 7.60	349.2	316.2	213.2	164	338.6	79.5	126.3	238.1	131.1	55.8	277.5	226.7	309.8	351.1	513
???	± 7.73	22.7	22.6	13.8	10.6	23	17.2	27.3	51	28.4	11	4.7	4.1	4.9		
Thymol	± 7.90	8744.6	8157.4	4762.6	3816	8068.2	3099.6	4990.7	9860.9	5251.7	2072.5	2767.5	2239.2	2885.1	3037.6	4351
????	± 8.19	29.2	28.3	16.7	12.3	28.8	18	27.6	51.9	26.8	11.5	6.7	5.6	7	6.4	9
????	± 8.33	282.2	280.6	163.8	126.5	280.4	185	295.1	566.6	300.4	121	60	48.4	57.8	57.5	79
6-n-Propyl-3-Methyl Phenol	± 8.40	142.6	120.7	77.2	68.7	133.4	33.3	50.9	104.8	57.6	22.7	56	51.5	65.6	63.8	85
2,6-Diisoprop.-3-Met. Phen.	± 8.55	26.2	25.4	15.1	11.8	26.3	17.6	27.2	51.9	28.2	11	4.7	4.7	5.4	5.1	7.4
5,3 Thymol isomer	± 8.67	908	895.5	503.3	390	893.5	591.9	969.1	1877.5	987.8	384.8	163.7	134.6	161.9	162.4	228
4,3 Thymol isomer	± 8.78	1529.9	1446.8	820.3	668	1481.5	497.9	814	1605.4	866.5	339.3	540.5	455.5	566	595	847
C-13 fraction (13.02)	± 8.83	1.6	2	1.4	0.8	2.1	1.3	2.5	4.3	2.3	2.1	1.9	2	2.1	2.2	2
????	± 9.22	27.9	27.6	17.8	13.2	29.9	29.5	46.9	84.2	44.9	20.6	3	3.6	3.5	3.7	4.4
????	± 9.48	36.3	35.5	16.9	15.9	36.6	25.8	41.3	76.6	41.5	17.3	6.7	5.8	7.1	6.3	10.3
????	± 9.60	7.1	6.4	4.4	2.9	7.8	2	8.9	15.9	8.5	4.3	2.3	1	1.8	1.9	1.2
????	± 10.30	16.7	17.6	14.5	8.8	19.7	19.4	32.5	59.3	32.3	12.8	1.9	0.8	1.7	0.3	1.5
????	± 10.70	4.8	4.2	3.5	2.7	4.4	3.8	7.1	12.5	6.7	11.2					
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1085.5	989.9	574.6	491.7	1028.7	414.4	651.8	1388.4	717.5	296.2	237	204.9	236.7	242.4	334.9
????	± 11.30															
????	± 11.80															
????	± 12.09															
????	± 12.21	11.6	8.6	5.1	6.1	10.9	4.9	8.4	18	7.5	3.9	3.2	2.8	4.1	3.6	3
5,6-Diisoprop.-3-Met. Phen.	± 12.70	71.8	66.9	39.6	33.5	73	34.4	53.5	104.6	56.4	24	17.6	15.7	17.7	19	26
Heavies	± 13.04	30.6	28.9	17.3	14.3	28.8	19.6	37.1	79.4	44.4	15.9	5	4.3	5.2	6	7
Heavies		11.2	10.6	10.9	15.6	13.7	20.7	33.1	26.4	20.4	22.3	13.8	8.9	10	28.6	15.3

Table 0.3: GC raw data for H-MFI-90 extrudates (cont.)

EXTRUDATE		EX-30	EX-31	EX-32	EX-33	EX-34	EX-35	EX-36	EX-37	EX-38	EX-39	EX-40	EX-41	EX-42	EX-43
Time on Stream		176:10:44	177:03:44	179:00:44	179:24:44	180:01:44	181:30:44	181:58:44	182:25:44	183:55:44	199:04:44	200:04:44	201:55:44	202:32:44	203:44:44
Entry Temperature		89	89	90	89	90	90	90	90	90	85	85	93	94	95
Temperature		275	276	276	275	276	275	275	274	275	275	275	275	275	275
WHSV		2.4	2.4	2.4	2.4	2.4	4.79	4.79	4.79	4.79	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.32	0.32	0.32	0.32	0.32	0.32	0.64	0.64	0.64	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	34.3	46.7	56.7	31.3	45.1	76.4	128	86.3	64.7	35.6	41.5	14.1	34.8	26.9
???	± 5.04														
phenol	± 5.26	4.7	6.1	8.1	4.3	5	2.9	3.7	2.7	1.6	5.6	6.6	2	4.5	3.7
o-Cresol	± 5.35	6.2	8.6	11.2	5.4	5.4	7.2	11.5	6.6	4.1	7.6	9.5	2.1	6.6	5.3
p-Cresol	± 5.60	60.3	82	103.8	54.4	74.3	75.1	113.5	70.4	44.8	67.8	82.4	22.2	56.9	48.4
m-Cresol	± 5.80	9689.2	13239.8	16730.8	8766.5	12116.2	12144.7	18506.9	11403.4	7224.7	11313.8	13714.2	3556.5	9526.4	8068.1
???	± 6.00	6	8.9	11.5	6.3	14	8.8	12.6	8	3.7	8.6	10.3	2.7	7.2	5.9
2,4-Xylenol	± 6.20	1.3	2.1	3.1	1.4	2	1.5	2.2	1	0.5	2.3	4	1	2.1	2
2,5-Xylenol	± 6.50	4.1	6.5	9.2	4.4	7	4.1	7.8	3.9	2.5	6.7	6.9	2.4	4.5	4.5
2,3-Xylenol	± 6.74	2	2.3	2.7	1.4	2	1.2	2.1	1.3	2.8	2.2	4.8	1.8	2.4	1.1
???	± 6.90														
???	± 7.03														
???	± 7.16	1.2	1.2	1.9	1.1	0.9	0.3	0.9	0.4	0.2	1.4	2.3	0.8	1.1	2.2
2-Isopropyl-4-methyl Phenol	± 7.30	22.1	30.5	38.3	21.5	28.2	14.8	22.8	14.7	9.3	39.6	51.3	14.5	33.4	30
???	± 7.49	1.2	1.5	1.1	1.6	1.2					2.2	2.6	0.8	1.2	1.1
Thymol isomer (2,3)	± 7.60	472.7	659.7	846.7	454.1	639	485.9	762.7	486.7	325	647.7	816.5	217.4	551.7	466.5
???	± 7.73	2.5	3.1	4.2	2	2.6					3.2	3.6	1.2	2.5	2.4
Thymol	± 7.90	2052.1	2887.8	3663.6	1874.5	2582	1173.7	1815.8	1135.8	736	3829.6	5018.2	1242.7	3151.2	2715.5
????	± 8.19	3.5	5	5.8	3.2	4	2.1	2.2	1.5		4.7	6.4	1.7	4	3.8
????	± 8.33	25.2	33.9	41.5	20.7	27	8.2	12.3	7.6	4	34.7	45.1	11.7	27.8	24.1
6-n-Propyl-3-Methyl Phenol	± 8.40	47.8	64.5	90.9	49.8	65	25.9	38.6	25.2	18	95.6	144.2	39.7	90.4	78.7
2,6-Diisoprop.-3-Met. Phen.	± 8.55	2.1	3.5	4.1	2.2	2					3.3	3.5	1.3	2.6	2.4
5,3 Thymol isomer	± 8.67	83.8	107.5	140.5	67	87	34.1	50.4	31.1	20	132.5	179.3	43.6	105.7	90.7
4,3 Thymol isomer	± 8.78	410.9	561.1	733.5	342.7	483	229	346.7	213.5	135	597.8	811.7	192.6	469.5	417
C-13 fraction (13.02)	± 8.83														
????	± 9.22														
????	± 9.48	3.4	4.8	6	2.8	4	1.9	1.7	2.5	1.1	4.4	6.3	2.7	3.7	2.4
????	± 9.60	1.5	1.3	0.3	0.7	0.3					2.2	1	1.1	1.4	0.9
????	± 10.30	0.9	2.1	3.3	1.3	2.2					0.9	0.9	0.6	1.3	0.6
????	± 10.70														
4,6-Diisoprop.-3-Met. Phen.	± 11.18	130.5	171.3	237.8	112.4	162	47.4	71.3	46	31	283.3	405.3	103.5	226.9	203
????	± 11.30														
????	± 11.80														
????	± 12.09														
????	± 12.21	2.6	2.2	3.7	2.9	3	2.8	1	1.9	4	3.8	5.5	1.3	4.3	2
5,6-Diisoprop.-3-Met. Phen.	± 12.70	11.7	16.2	22.8	10	16	7.9	9.6	6.6	4.2	19.1	28	7	15.5	15
Heavies	± 13.04	1.6	2.2	4.4	2.1	2	1.4	1.1	1.3	1	5.4	7.7	1.1	3.3	3
Heavies		11.4	18	13.4	11.4	12	11.5	15.1	8.7	10.4	8.9	13.9	9.5	10.3	9.9

Appendix: Simulated washcoating GC product analysis

Table 0.4: Product composition (%) for H-MFI-90 extrudates

EXTRUDATE		EX-1	EX-2	EX-3	EX-4	EX-5	EX-6	EX-7	EX-8	EX-9	EX-10	EX-11	EX-12	EX-13	EX-14
Time on Stream		1:22	2:22	7:26	9:26	11:30	13:27	18:08	30:30	37:20	57:55	67:10	77:10	80:09	83:05
Entry Temperature		90	90	91	91	92	93	93	93	92	91	93	93	86	93
Temperature		275	275	275	274	275	274	275	275	275	275	274	275	275	276
WHSV		1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	-	-	-	-	-	-	0.08	0.10	0.11	0.09	0.12	0.11	0.11	0.12
???	± 5.04	0.34	0.10	0.04	0.06	0.07	0.08	0.04	0.02	0.01	0.01	0.01	0.01	0.01	0.01
phenol	± 5.26	-	-	0.02	0.00	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.03
o-Cresol	± 5.35	0.16	0.38	0.09	0.07	0.01	0.04	0.04	0.05	0.04	0.05	0.04	0.05	0.05	0.05
p-Cresol	± 5.60	3.58	1.23	0.55	0.43	0.41	0.45	0.43	0.44	0.41	0.45	0.46	0.44	0.44	0.44
m-Cresol	± 5.80	75.56	59.25	48.97	48.56	46.64	49.68	51.35	54.68	55.35	63.43	64.90	64.43	65.80	66.18
???	± 6.00	0.09	0.05	0.03	0.03	0.03	0.02	0.03	0.03	0.04	0.03	0.03	0.04	0.03	0.03
2,4-Xylenol	± 6.20	0.48	0.24	0.12	0.07	0.05	0.05	0.04	0.03	0.03	0.03	0.03	0.02	0.03	0.03
2,5-Xylenol	± 6.50	0.15	0.11	0.08	0.06	0.06	0.07	0.05	0.06	0.05	0.04	0.05	0.05	0.04	0.04
2,3-Xylenol	± 6.74	0.05	0.13	0.04	0.04	0.03	0.04	0.03	0.02	0.03	0.02	0.02	0.02	0.01	0.02
???	± 6.90	0.34	0.20	0.09	0.06	0.03	0.04	0.03	0.03	0.02	0.01	0.02	0.01	0.01	0.01
???	± 7.03	-	-	-	-	-	0.01	0.01	-	0.01	0.00	-	0.00	-	-
???	± 7.16	0.60	0.42	0.19	0.10	0.09	0.07	0.05	0.04	0.03	0.02	0.02	0.02	0.02	0.02
2-Isopropyl-4-methyl Phenol	± 7.30	0.52	0.43	0.36	0.33	0.34	0.32	0.31	0.29	0.28	0.24	0.24	0.23	0.23	0.24
???	± 7.49	0.14	0.08	0.04	0.05	0.07	0.06	0.04	0.04	0.03	0.02	0.02	0.02	0.02	0.02
Thymol isomer (2,3)	± 7.60	0.27	0.35	0.64	0.96	1.16	1.20	1.38	1.56	1.80	1.67	1.70	1.73	1.85	1.83
???	± 7.73	0.62	0.44	0.25	0.17	0.16	0.14	0.11	0.09	0.07	0.06	0.06	0.05	0.04	0.04
Thymol	± 7.90	1.02	17.32	27.25	30.58	32.07	31.04	30.58	29.07	28.68	24.30	23.21	23.36	23.02	22.66
????	± 8.19	0.76	0.48	0.28	0.21	0.19	0.18	0.13	0.11	0.10	0.08	0.07	0.71	0.06	0.07
????	± 8.33	3.03	3.02	2.54	1.96	1.82	1.65	1.36	1.08	0.87	0.70	0.65	0.59	0.52	0.52
6-n-Propyl-3-Methyl Phenol	± 8.40	0.07	0.07	0.21	0.36	0.45	0.27	0.54	0.54	0.59	0.41	0.39	0.41	0.39	0.40
2,6-Diisoprop.-3-Met. Phen.	± 8.55	1.30	0.03	0.45	0.28	0.24	0.21	0.17	0.12	0.10	0.07	0.07	0.06	0.05	0.05
5,3 Thymol isomer	± 8.67	4.73	6.28	6.37	5.17	4.95	4.31	3.77	3.10	2.74	2.00	1.96	1.75	1.62	1.60
4,3 Thymol isomer	± 8.78	1.54	2.64	4.11	4.53	4.88	4.47	4.50	4.20	4.49	3.70	3.40	3.50	3.43	3.38
C-13 fraction (13.02)	± 8.83	0.20	0.08	0.03	0.02	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.00
????	± 9.22	0.07	0.90	0.65	0.36	0.29	0.23	0.17	0.12	0.08	0.04	0.06	0.04	0.03	0.04
????	± 9.48	0.59	0.52	0.33	0.22	0.20	0.18	0.14	0.11	0.10	0.07	0.06	0.06	0.06	0.04
????	± 9.60	0.21	0.19	0.10	0.05	0.04	0.03	0.03	0.02	0.02	0.01	0.01	0.01	0.01	0.02
????	± 10.30	1.30	1.31	0.71	0.30	0.23	0.18	0.11	0.07	0.06	0.03	0.03	0.02	0.02	0.01
????	± 10.70	0.36	0.28	0.14	0.05	0.04	0.04	0.03	0.02	0.01	0.01	0.01	0.00	0.01	0.01
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.87	1.90	3.68	3.99	4.40	3.90	3.80	3.42	3.33	2.08	2.03	1.95	1.83	1.85
????	± 11.30	0.08	0.01	0.02	0.01	0.01	-	-	-	-	-	-	-	-	-
????	± 11.80	0.29	0.23	0.08	0.02	0.02	-	-	-	-	-	-	-	-	-
????	± 12.09	0.03	0.10	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.03	0.06	0.10	0.07	0.07	0.06	0.08	0.06	0.06	0.04	0.03	0.04	0.02	0.03
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.16	0.28	0.37	0.27	0.22	0.34	0.33	0.28	0.27	0.17	0.16	0.15	0.14	0.14
Heavies	± 13.04	0.34	0.06	0.51	0.20	0.48	0.21	0.13	0.10	0.08	0.05	0.06	0.04	0.04	0.04
Heavies		0.11	0.85	0.55	0.34	0.28	0.46	0.14	0.12	0.08	0.05	0.08	0.05	0.03	0.06

Table 0.5: Product composition (%) for H-MFI-90 extrudates (cont.)

EXTRUDATE		EX-15	EX-16	EX-17	EX-18	EX-19	EX-20	EX-21	EX-22	EX-23	EX-24	EX-25	EX-26	EX-27	EX-28	EX-29
Time on Stream		115:13	117:12	119:12	121:13	125:06	144:01	146:23	150:07	159:10	161:09	171:12	172:05	173:19	174:08	174:34
Entry Temperature		94	94	94	94	92	92	93	93	93	92	94	96	96	95	95
Temperature		275	275	275	275	275	275	276	275	275	276	275	274	274	275	275
WHSV		0.6	0.6	0.6	0.6	0.6	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.08	0.08	0.08	0.08	0.08	0.04	0.04	0.04	0.04	0.04	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.06	0.06	0.08	0.10	0.07	0.03	0.03	0.03	0.04	0.04	0.13	0.14	0.13	0.13	0.13
???	± 5.04	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.03	0.02	-	-	-	-	0.03
phenol	± 5.26	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.03	0.03	0.03	0.02	0.04
o-Cresol	± 5.35	0.05	0.05	0.05	0.06	0.05	0.05	0.05	0.06	0.05	0.05	0.05	0.05	0.05	0.05	0.05
p-Cresol	± 5.60	0.41	0.43	0.43	0.42	0.42	0.46	0.45	0.44	0.43	0.46	0.47	0.47	0.47	0.47	0.47
m-Cresol	± 5.80	57.26	59.48	59.74	57.01	57.94	53.13	53.27	51.96	51.76	52.88	72.00	70.93	72.82	73.83	74.27
???	± 6.00	0.03	-	-	-	0.04	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	0.07
2,4-Xylenol	± 6.20	0.04	0.04	0.07	0.03	0.04	0.07	0.07	0.06	0.06	0.06	0.02	0.02	0.02	0.01	0.02
2,5-Xylenol	± 6.50	0.05	0.05	0.03	0.05	0.05	0.07	0.07	0.07	0.07	0.03	0.04	0.04	0.04	0.03	0.04
2,3-Xylenol	± 6.74	0.01	0.01	0.01	0.02	0.01	0.03	0.02	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
???	± 6.90	0.03	0.02	0.02	0.00	0.02	0.05	0.06	0.03	0.05	0.04	0.00	0.01	-	-	-
???	± 7.03	-	-	-	-	-	-	-	0.01	-	-	-	-	-	-	-
???	± 7.16	0.04	0.03	0.04	0.04	0.04	0.07	0.09	0.07	0.08	0.07	0.02	0.02	0.01	0.01	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.29	0.28	0.28	0.30	0.28	0.37	0.37	0.37	0.37	0.38	0.22	0.21	0.20	0.18	0.18
???	± 7.49	0.03	0.03	0.03	0.03	0.03	0.05	0.04	0.04	0.07	0.04	0.01	0.02	0.01	0.01	0.01
Thymol isomer (2,3)	± 7.60	1.15	1.06	1.21	1.24	1.17	0.75	0.73	0.72	0.75	0.78	1.89	1.96	1.96	2.03	2.04
???	± 7.73	0.07	0.08	0.08	0.08	0.08	0.16	0.16	0.15	0.16	0.15	0.03	0.04	0.03	0.03	0.04
Thymol	± 7.90	28.86	27.24	27.02	28.82	27.93	29.12	28.98	29.92	30.04	29.08	18.84	19.37	18.27	17.55	17.33
????	± 8.19	0.10	0.09	0.09	0.09	0.10	0.17	0.16	0.16	0.15	0.16	0.05	0.05	0.04	0.04	0.04
????	± 8.33	0.93	0.94	0.93	0.96	0.97	1.74	1.71	1.72	1.72	1.70	0.41	0.42	0.37	0.33	0.31
6-n-Propyl-3-Methyl Phenol	± 8.40	0.36	0.31	0.33	0.39	0.35	0.24	0.22	0.24	0.25	0.24	0.29	0.34	0.32	0.28	0.26
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.09	0.08	0.09	0.09	0.09	0.17	0.16	0.16	0.16	0.15	0.03	0.04	0.03	0.03	0.03
5,3 Thymol isomer	± 8.67	3.00	2.99	2.86	2.95	3.09	5.56	5.63	5.70	5.65	5.40	1.11	1.16	1.03	0.94	0.91
4,3 Thymol isomer	± 8.78	3.84	3.68	3.54	3.84	3.90	3.56	3.60	3.71	3.77	3.62	2.80	3.00	2.73	2.62	2.57
C-13 fraction (13.02)	± 8.83	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
????	± 9.22	0.07	0.07	0.08	0.08	0.08	0.21	0.21	0.19	0.20	0.22	0.02	0.02	0.02	0.02	0.01
????	± 9.48	0.09	0.09	0.07	0.09	0.10	0.18	0.18	0.18	0.18	0.18	0.03	0.04	0.03	0.03	0.03
????	± 9.60	0.02	0.02	0.02	0.02	0.02	0.01	0.04	0.04	0.04	0.05	0.01	0.01	0.01	0.01	0.00
????	± 10.30	0.04	0.04	0.06	0.05	0.05	0.14	0.14	0.14	0.14	0.14	0.01	0.01	0.01	0.00	0.00
????	± 10.70	0.01	0.01	0.02	0.02	0.01	0.03	0.03	0.03	0.03	0.12	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	2.73	2.52	2.48	2.83	2.71	2.96	2.88	3.21	3.12	3.16	1.23	1.35	1.14	1.07	1.02
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.03	0.02	0.02	0.04	0.03	0.04	0.04	0.04	0.03	0.04	0.02	0.02	0.02	0.02	0.01
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.18	0.17	0.17	0.19	0.19	0.25	0.24	0.24	0.25	0.26	0.09	0.10	0.09	0.08	0.08
Heavies	± 13.04	0.08	0.07	0.07	0.08	0.08	0.14	0.16	0.18	0.19	0.17	0.03	0.03	0.03	0.03	0.02
Heavies		0.03	0.03	0.05	0.09	0.04	0.15	0.15	0.06	0.09	0.24	0.07	0.06	0.05	0.13	0.05

Table 0.6: Product composition (%) for H-MFI-90 extrudates (cont.)

EXTRUDATE		EX-30	EX-31	EX-32	EX-33	EX-34	EX-35	EX-36	EX-37	EX-38	EX-39	EX-40	EX-41	EX-42	EX-43
Time on Stream		176:10:44	177:03:44	179:00:44	179:24:44	180:01:44	181:30:44	181:58:44	182:25:44	183:55:44	199:04:44	200:04:44	201:55:44	202:32:44	203:44:44
Entry Temperature		89	89	90	89	90	90	90	90	90	85	85	93	94	95
Temperature		275	276	276	275	276	275	275	274	275	275	275	275	275	275
WHSV		2.4	2.4	2.4	2.4	2.4	4.79	4.79	4.79	4.79	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.32	0.32	0.32	0.32	0.32	0.64	0.64	0.64	0.64	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.21	0.21	0.20	0.21	0.22	0.40	0.44	0.48	0.57	0.17	0.16	0.21	0.20	0.18
???	± 5.04	-	-	-	-	0.03	-	-	-	-	-	-	-	-	-
phenol	± 5.26	0.03	0.03	0.03	0.03	0.03	0.02	0.01	0.02	0.01	0.03	0.03	0.03	0.03	0.02
o-Cresol	± 5.35	0.05	0.05	0.05	0.05	0.05	0.05	0.06	0.05	0.05	0.05	0.05	0.04	0.05	0.05
p-Cresol	± 5.60	0.50	0.50	0.50	0.50	0.50	0.55	0.54	0.55	0.55	0.45	0.44	0.46	0.45	0.45
m-Cresol	± 5.80	81.08	80.79	80.61	81.00	81.01	88.99	88.85	88.63	88.25	74.47	72.90	73.47	74.85	74.50
???	± 6.00	0.04	0.04	0.04	0.04	0.07	0.05	0.05	0.05	0.03	0.04	0.04	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.02	0.02	0.01	0.01
2,5-Xylenol	± 6.50	0.03	0.03	0.03	0.03	0.04	0.02	0.03	0.02	0.02	0.03	0.03	0.04	0.03	0.03
2,3-Xylenol	± 6.74	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.03	0.01	0.02	0.03	0.01	0.01
???	± 6.90	-	-	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.02
2-Isopropyl-4-methyl Phenol	± 7.30	0.14	0.14	0.14	0.15	0.14	0.08	0.08	0.09	0.09	0.20	0.21	0.23	0.20	0.21
???	± 7.49	0.01	0.01	0.00	0.01	0.01	-	-	-	-	0.01	0.01	0.01	0.01	0.01
Thymol isomer (2,3)	± 7.60	2.71	2.76	2.80	2.88	2.93	2.44	2.51	2.59	2.72	2.92	2.98	3.08	2.97	2.95
???	± 7.73	0.01	0.01	0.01	0.01	0.01	-	-	-	-	0.01	0.01	0.02	0.01	0.02
Thymol	± 7.90	11.78	12.09	12.11	11.88	11.84	5.90	5.98	6.05	6.17	17.29	18.30	17.61	16.98	17.20
????	± 8.19	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02
????	± 8.33	0.14	0.14	0.14	0.13	0.12	0.04	0.04	0.04	0.03	0.16	0.16	0.17	0.15	0.15
6-n-Propyl-3-Methyl Phenol	± 8.40	0.21	0.21	0.23	0.24	0.23	0.10	0.10	0.10	0.11	0.33	0.40	0.43	0.37	0.38
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.01	0.01	0.01	0.01	0.01	-	-	-	-	0.01	0.01	0.02	0.01	0.02
5,3 Thymol isomer	± 8.67	0.48	0.45	0.46	0.42	0.40	0.17	0.17	0.17	0.17	0.60	0.65	0.62	0.57	0.57
4,3 Thymol isomer	± 8.78	1.79	1.79	1.84	1.65	1.69	0.88	0.87	0.87	0.86	2.05	2.25	2.08	1.93	2.01
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.22	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.48	0.01	0.02	0.02	0.01	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.03	0.02	0.01
????	± 9.60	0.01	0.00	0.00	0.00	0.00	-	-	-	-	0.01	0.00	0.01	0.01	0.00
????	± 10.30	0.00	0.01	0.01	0.01	0.01	-	-	-	-	0.00	0.00	0.01	0.01	0.00
????	± 10.70	-	-	-	-	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.57	0.55	0.60	0.54	0.57	0.18	0.18	0.19	0.20	0.97	1.12	1.12	0.93	0.98
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.03	0.01	0.02	0.01	0.02	0.01
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.05	0.05	0.06	0.05	0.06	0.03	0.02	0.03	0.03	0.07	0.08	0.08	0.06	0.07
Heavies	± 13.04	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.01	0.01	0.01
Heavies		0.05	0.06	0.03	0.05	0.04	0.04	0.04	0.04	0.07	0.03	0.04	0.10	0.04	0.05

Table 0.7: Conversion, selectivity and yield data for H-MFI-90 extrudates

EXTRUDATE	EX-1	EX-2	EX-3	EX-4	EX-5	EX-6	EX-7	EX-8	EX-9	EX-10	EX-11	EX-12	EX-13	EX-14
Time on Stream	1:22:38	2:22:48	7:26:48	9:26:48	11:30:48	13:27:48	18:08:48	30:30:48	37:20:48	57:55:46	67:10:46	77:10:46	80:09:46	83:05:44
Entry Temperature	90	90	91	91	92	93	93	93	92	91	93	93	86	93
Temperature	275	275	275	274	275	274	275	275	275	275	274	275	275	276
WHSV	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	24.44	40.75	51.03	51.44	53.36	50.32	48.65	45.32	44.65	36.57	35.10	35.57	34.20	33.82
Thymol Selectivity	4.16	42.49	53.41	59.46	60.10	61.68	62.86	64.13	64.23	66.43	66.14	65.67	67.32	67.02
Thymol Yield	1.02	17.32	27.25	30.58	32.07	31.04	30.58	29.07	28.68	24.30	23.21	23.36	23.02	22.66
S3-isopropyl-5-methylphenol	**19.36**	**15.42**	**12.49**	**10.06**	**9.27**	**8.57**	**7.74**	**6.85**	**6.14**	**5.47**	**5.58**	**4.91**	**4.73**	**4.73**
Y3-methyl-5-isopropylphenol	4.73	6.28	6.37	5.17	4.95	4.31	3.77	3.10	2.74	2.00	1.96	1.75	1.62	1.60
S4-isopropyl-3-methylphenol	**6.32**	**6.48**	**8.06**	**8.81**	**9.15**	**8.88**	**9.24**	**9.27**	**10.06**	**10.10**	**9.70**	**9.83**	**10.04**	**10.00**
Y3-methyl-4-isopropylphenol	1.54	2.64	4.11	4.53	4.88	4.47	4.50	4.20	4.49	3.70	3.40	3.50	3.43	3.38
S2-isopropyl-3-methylphenol	**1.11**	**0.85**	**1.26**	**1.87**	**2.17**	**2.39**	**2.85**	**3.45**	**4.04**	**4.57**	**4.83**	**4.87**	**5.40**	**5.40**
Y3-methyl-2-isopropylphenol	0.27	0.35	0.64	0.96	1.16	1.20	1.38	1.56	1.80	1.67	1.70	1.73	1.85	1.83
Thymol	13.45	65.13	71.01	74.13	74.48	75.66	76.02	76.61	76.04	76.73	76.68	77.00	76.95	76.90
3-methyl-5-isopropylphenol	62.55	23.63	16.61	12.54	11.49	10.51	9.36	8.18	7.27	6.31	6.47	5.75	5.41	5.42
3-methyl-2-isopropylphenol	20.42	9.93	10.71	10.99	11.34	10.89	11.18	11.08	11.91	11.67	11.25	11.53	11.47	11.48
3-methyl-4-isopropylphenol	3.58	1.30	1.67	2.34	2.69	2.94	3.44	4.12	4.78	5.28	5.60	5.72	6.17	6.20
STotal.Isomer	**30.95**	**65.24**	**75.22**	**80.20**	**80.70**	**81.52**	**82.69**	**83.70**	**84.47**	**86.57**	**86.25**	**85.28**	**87.48**	**87.16**
YTotal.Isomer	7.56	26.58	38.38	41.25	43.06	41.02	40.23	37.94	37.71	31.66	30.27	30.34	29.92	29.47
Slights	9.70	4.06	1.87	1.44	1.28	1.30	1.24	1.21	1.17	1.16	1.23	1.19	1.13	1.18
Ylights	2.37	1.65	0.95	0.74	0.68	0.65	0.60	0.55	0.52	0.42	0.43	0.42	0.39	0.40
SC-10	18.01	9.65	6.03	4.54	4.06	3.90	3.30	2.85	2.35	2.30	2.22	3.78	1.84	1.85
YC-10	4.40	3.93	3.08	2.34	2.17	1.96	1.61	1.29	1.05	0.84	0.78	1.34	0.63	0.63
Sdi-isopropylated	5.89	5.66	9.34	9.37	10.40	9.38	9.84	9.57	9.56	7.41	7.49	7.17	7.01	7.15
Ydi-isopropylated	1.44	2.31	4.76	4.82	5.55	4.72	4.79	4.34	4.27	2.71	2.63	2.55	2.40	2.42
Sheavies	0.44	2.09	1.07	0.65	0.52	0.91	0.29	0.26	0.18	0.13	0.24	0.14	0.10	0.17
Yheavies	0.11	0.85	0.55	0.34	0.28	0.46	0.14	0.12	0.08	0.05	0.08	0.05	0.03	0.06
Sether	1.41	0.24	0.11	0.13	0.15	0.20	0.20	0.26	0.31	0.33	0.40	0.39	0.41	0.44
Yether	0.34	0.10	0.06	0.06	0.08	0.10	0.10	0.12	0.14	0.12	0.14	0.14	0.14	0.15

Table 0.8: Conversion, selectivity and yield data for H-MFI-90 extrudates (cont.)

EXTRUDATE	EX-15	EX-16	EX-17	EX-18	EX-19	EX-20	EX-21	EX-22	EX-23	EX-24	EX-25	EX-26	EX-27	EX-28	EX-29
Time on Stream	115:13:44	117:12:44	119:12:44	121:13:44	125:06:44	144:01:44	146:23:44	150:07:44	159:10:44	161:09:44	171:12:44	172:05:44	173:19:44	174:08:44	174:34:44
Entry Temperature	94	94	94	94	92	92	93	93	93	92	94	96	96	95	95
Temperature	275	275	275	275	275	275	276	275	275	276	275	274	274	275	275
WHSV	0.6	0.6	0.6	0.6	0.6	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.08	0.08	0.08	0.08	0.08	0.04	0.04	0.04	0.04	0.04	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	42.74	40.52	40.26	42.99	42.06	46.87	46.73	48.04	48.24	47.12	28.00	29.07	27.18	26.17	25.73
Thymol Selectivity	67.52	67.22	67.11	67.03	66.42	62.13	62.02	62.29	62.27	61.71	67.29	66.64	67.21	67.07	67.38
Thymol Yield	28.86	27.24	27.02	28.82	27.93	29.12	28.98	29.92	30.04	29.08	18.84	19.37	18.27	17.55	17.33
S3-isopropyl-5-methylphenol	**7.01**	**7.38**	**7.09**	**6.85**	**7.36**	**11.86**	**12.04**	**11.86**	**11.71**	**11.46**	**3.98**	**4.01**	**3.77**	**3.59**	**3.53**
Y3-methyl-5-isopropylphenol	3.00	2.99	2.86	2.95	3.09	5.56	5.63	5.70	5.65	5.40	1.11	1.16	1.03	0.94	0.91
S4-isopropyl-3-methylphenol	**8.99**	**9.07**	**8.80**	**8.93**	**9.28**	**7.59**	**7.70**	**7.72**	**7.82**	**7.69**	**10.00**	**10.32**	**10.03**	**10.00**	**9.98**
Y3-methyl-4-isopropylphenol	3.84	3.68	3.54	3.84	3.90	3.56	3.60	3.71	3.77	3.62	2.80	3.00	2.73	2.62	2.57
S2-isopropyl-3-methylphenol	**2.70**	**2.61**	**3.00**	**2.88**	**2.79**	**1.59**	**1.57**	**1.50**	**1.55**	**1.66**	**6.75**	**6.75**	**7.22**	**7.75**	**7.94**
Y3-methyl-2-isopropylphenol	1.15	1.06	1.21	1.24	1.17	0.75	0.73	0.72	0.75	0.78	1.89	1.96	1.96	2.03	2.04
Thymol	78.31	77.91	78.03	78.22	77.37	74.69	74.43	74.71	74.70	74.78	76.45	75.98	76.17	75.87	75.85
3-methyl-5-isopropylphenol	8.13	8.55	8.25	7.99	8.57	14.26	14.45	14.23	14.05	13.89	4.52	4.57	4.27	4.06	3.97
3-methyl-2-isopropylphenol	10.43	10.52	10.23	10.42	10.81	9.13	9.24	9.26	9.38	9.32	11.36	11.76	11.37	11.31	11.24
3-methyl-4-isopropylphenol	3.13	3.02	3.49	3.36	3.25	1.92	1.88	1.80	1.86	2.01	7.67	7.69	8.18	8.77	8.94
STotal.Isomer	**86.22**	**86.27**	**86.01**	**85.70**	**85.84**	**83.18**	**83.33**	**83.37**	**83.35**	**82.52**	**88.02**	**87.71**	**88.23**	**88.41**	**88.83**
YTotal.Isomer	36.85	34.96	34.63	36.84	36.10	38.99	38.94	40.05	40.21	38.88	24.65	25.50	23.98	23.14	22.85
Slights	1.21	1.13	1.19	1.09	1.18	1.54	1.57	1.44	1.56	1.45	1.26	1.27	1.23	1.14	1.30
Ylights	0.52	0.46	0.48	0.47	0.50	0.72	0.73	0.69	0.75	0.68	0.35	0.37	0.33	0.30	0.33
SC-10	2.58	2.73	2.74	2.62	2.73	4.41	4.35	4.23	4.22	4.27	1.74	1.73	1.62	1.41	1.36
YC-10	1.10	1.11	1.10	1.13	1.15	2.07	2.03	2.03	2.03	2.01	0.49	0.50	0.44	0.37	0.35
Sdi-isopropylated	7.82	7.56	7.60	8.13	7.92	7.65	7.50	8.06	7.90	8.13	5.84	6.26	5.76	5.57	5.34
Ydi-isopropylated	3.34	3.07	3.06	3.50	3.33	3.59	3.51	3.87	3.81	3.83	1.64	1.82	1.57	1.46	1.37
Sheavies	0.07	0.07	0.12	0.21	0.09	0.32	0.31	0.13	0.18	0.51	0.26	0.20	0.18	0.48	0.18
Yheavies	0.03	0.03	0.05	0.09	0.04	0.15	0.15	0.06	0.09	0.24	0.07	0.06	0.05	0.13	0.05
Sether	0.20	0.20	0.25	0.27	0.21	0.13	0.12	0.11	0.15	0.09	0.56	0.56	0.57	0.58	0.78
Yether	0.08	0.08	0.10	0.12	0.09	0.06	0.06	0.05	0.07	0.04	0.16	0.16	0.16	0.15	0.20

Table 0.9: Conversion, selectivity and yield data for H-MFI-90 extrudates (cont.)

EXTRUDATE	EX-30	EX-31	EX-32	EX-33	EX-34	EX-35	EX-36	EX-37	EX-38	EX-39	EX-40	EX-41	EX-42	EX-43
Time on Stream	176:10:44	177:03:44	179:00:44	179:24:44	180:01:44	181:30:44	181:58:44	182:25:44	183:55:44	199:04:44	200:04:44	201:55:44	202:32:44	203:44:44
Entry Temperature	89	89	90	89	90	90	90	90	90	85	85	93	94	95
Temperature	275	276	276	275	276	275	275	274	275	275	275	275	275	275
WHSV	2.4	2.4	2.4	2.4	2.4	4.79	4.79	4.79	4.79	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)	0.32	0.32	0.32	0.32	0.32	0.64	0.64	0.64	0.64	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	18.92	19.21	19.39	19.00	18.99	11.01	11.15	11.37	11.75	25.53	27.10	26.53	25.15	25.50
Thymol Selectivity	62.27	62.93	62.44	62.52	62.34	53.57	53.61	53.23	52.46	67.70	67.51	66.38	67.53	67.46
Thymol Yield	11.78	12.09	12.11	11.88	11.84	5.90	5.98	6.05	6.17	17.29	18.30	17.61	16.98	17.20
S3-isopropyl-5-methylphenol	**2.54**	**2.34**	**2.39**	**2.23**	**2.10**	**1.56**	**1.49**	**1.46**	**1.43**	**2.34**	**2.41**	**2.33**	**2.27**	**2.25**
Y3-methyl-5-isopropylphenol	0.48	0.45	0.46	0.42	0.40	0.17	0.17	0.17	0.17	0.60	0.65	0.62	0.57	0.57
S4-isopropyl-3-methylphenol	**9.49**	**9.30**	**9.51**	**8.70**	**8.87**	**7.95**	**7.79**	**7.61**	**7.32**	**8.04**	**8.31**	**7.83**	**7.66**	**7.88**
Y3-methyl-4-isopropylphenol	1.79	1.79	1.84	1.65	1.69	0.88	0.87	0.87	0.86	2.05	2.25	2.08	1.93	2.01
S2-isopropyl-3-methylphenol	**14.34**	**14.37**	**14.43**	**15.15**	**15.43**	**22.18**	**22.52**	**22.81**	**23.17**	**11.45**	**10.98**	**11.61**	**11.82**	**11.59**
Y3-methyl-2-isopropylphenol	2.71	2.76	2.80	2.88	2.93	2.44	2.51	2.59	2.72	2.92	2.98	3.08	2.97	2.95
Thymol	70.25	70.75	70.33	70.57	70.25	62.83	62.77	62.54	62.18	75.61	75.67	75.30	75.64	75.64
3-methyl-5-isopropylphenol	2.87	2.63	2.70	2.52	2.37	1.83	1.74	1.71	1.69	2.62	2.70	2.64	2.54	2.53
3-methyl-2-isopropylphenol	10.70	10.46	10.72	9.82	10.00	9.33	9.12	8.95	8.68	8.98	9.31	8.88	8.58	8.84
3-methyl-4-isopropylphenol	16.18	16.16	16.25	17.09	17.39	26.01	26.37	26.80	27.46	12.79	12.31	13.17	13.24	12.99
STotal.Isomer	**88.64**	**88.95**	**88.78**	**88.60**	**88.74**	**85.26**	**85.41**	**85.11**	**84.38**	**89.54**	**89.22**	**88.16**	**89.28**	**89.18**
YTotal.Isomer	16.77	17.08	17.21	16.83	16.85	9.39	9.52	9.68	9.92	22.86	24.18	23.38	22.45	22.74
Slights	1.28	1.29	1.29	1.40	1.49	1.57	1.60	1.53	1.51	1.24	1.24	1.43	1.24	1.30
Ylights	0.24	0.25	0.25	0.27	0.28	0.17	0.18	0.17	0.18	0.32	0.33	0.38	0.31	0.33
SC-10	0.95	0.92	0.88	0.86	0.75	0.47	0.43	0.43	0.29	0.75	0.74	0.78	0.74	0.75
YC-10	0.18	0.18	0.17	0.16	0.14	0.05	0.05	0.05	0.03	0.19	0.20	0.21	0.18	0.19
Sdi-isopropylated	4.42	4.21	4.62	4.42	4.50	2.87	2.71	2.82	2.94	5.43	5.99	6.15	5.48	5.67
Ydi-isopropylated	0.84	0.81	0.89	0.84	0.85	0.32	0.30	0.32	0.35	1.39	1.62	1.63	1.38	1.44
Sheavies	0.26	0.30	0.17	0.29	0.22	0.40	0.34	0.31	0.56	0.12	0.14	0.39	0.17	0.19
Yheavies	0.05	0.06	0.03	0.05	0.04	0.04	0.04	0.04	0.07	0.03	0.04	0.10	0.04	0.05
Sether	1.24	1.21	1.16	1.25	1.46	3.80	4.08	4.38	4.96	0.76	0.68	0.90	0.88	0.80
Yether	0.23	0.23	0.22	0.24	0.28	0.42	0.46	0.50	0.58	0.20	0.18	0.24	0.22	0.20

Table 0.10: GC raw data for simulated washcoating

		WC-1	WC-2	WC-3	WC-4	WC-5	WC-6	WC-7	WC-8	WC-9	WC-10
Time on Stream		07:10:44	08:10:44	09:00:44	11:00:44	11:50:44	14:30:44	17:30:44	31:40:44	33:00:44	35:00:44
Entry Temperature		103	103	104	105	105	105	105	101	104	103
Temperature		274	277	278	276	275	275	275	275	275	275
WHSV		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	5.7	30.4	22.7	23.9	34.5	33.3	33.8	43.6	38.3	44.3
???	± 5.04	11.03	3.8	2.2	1.8	2.4	1.3	1.2	1.7	1.4	1.6
phenol	± 5.26	1.2	5.6	3.9	4.4	6.6		6.3	9.3	7.3	8.6
o-Cresol	± 5.35	69.6	14.5	8.3	7.9	11.6	10.2	9.3	11.1	10.1	11.1
p-Cresol	± 5.60	313	98.1	65.1	61.1	86.1	81.6	75.5	96.9	77.9	84.8
m-Cresol	± 5.80	12827.3	12504.4	8606.3	8556.5	12150.4	11740.3	10974.6	14250.1	11726.4	12998.7
???	± 6.00	8.1	18.1	17.7	8.1	7.9	14.6	13.8	28.4	14.1	9.3
2,4-Xylenol	± 6.20	17.5	18.2	16.7	7.8	10.6	8.3	7.6	15.6	5.9	5.9
2,5-Xylenol	± 6.50	10.9	10.2	15.6	9.2	13.7	12.3	8	17.5	8.9	8
2,3-Xylenol	± 6.74	10.9	15.8	6.4	6.4	8.7	7.2	9.8	8.3	4.9	3
???	± 6.90	13.2	9.3	6.4	5	6.8	5.6	6.9	4.5	3.5	5.5
???	± 7.03		3.1	1.8	1.4	1.6	1.2	1.6	1.1	2.1	3.9
???	± 7.16	25	20.9	12.9	8.3	12.7	10.5	7.7	7.1	4.5	5.4
2-Isopropyl-4-methyl Phenol	± 7.30	35	79.2	57.7	48.1	70.4	63.7	56.3	59	46	49.2
???	± 7.49		19.4	12.2	8.3	12.8	10.2	9.6	11.9	6.4	5.9
Thymol isomer (2,3)	± 7.60	116.9	446.9	343.1	363.5	569.5	534.4	525.7	669	533.8	625.8
???	± 7.73	45.9	35	24.5	1702	23.3	19.4	15.2	32.9	9.5	9.6
Thymol	± 7.90	3147.2	8959	6802	5748.6	8627.7	7654.9	6696.4	6976.7	5233	5550.5
????	± 8.19		42.1	31.2	21.3	31.6	27	22.5	19	14.1	13.8
????	± 8.33	397.1	354.8	264.5	181.8	255	212.5	166	138.6	98.4	98.2
6-n-Propyl-3-Methyl Phenol	± 8.40	43.9	210.2	164.9	164.5	268	222	212.6	239.4	176.6	189.7
2,6-Diisoprop.-3-Met. Phen.	± 8.55		43.1	30.2	19.9	27	21.5	16.7	14.9	8.6	8.7
5,3 Thymol isomer	± 8.67	478.4	869.5	626.4	461.8	705.5	594	494.6	451.3	322	343.5
4,3 Thymol isomer	± 8.78	507.1	1457.3	1092.7	958.5	1507	1310.4	1190.5	1271.2	934.4	999.1
C-13 fraction (13.02)	± 8.83	8.5	4.2	2.3	1.7	2.8	2.2	1.9	1.8	1.2	1
????	± 9.22	88.7	79.4	50.6	30.9	44.5	31.4	25.6	18	11.5	13.5
????	± 9.48	44.5	43.7	31.1	21.6	32.5	26.1	21.7	18.2	13.5	14.6
????	± 9.60	13.4	12.4	8	6.5	7.7	6.3	6.7	13.8	3	4.7
????	± 10.30	26	55.4	34.6	19.9	29.3	21.7	16	10.3	7.2	8.3
????	± 10.70	99.5	13	5.5	4.3	7.4	7.4	5.8	12	3.5	2.6
4,6-Diisoprop.-3-Met. Phen.	± 11.18	397.2	1415.7	1035.8	832.9	1404.4	1091.7	976.8	875.9	673.8	685.7
????	± 11.30	5							10.3		
????	± 11.80	2.1	1.7								
????	± 12.09	6.7	2.6								
????	± 12.21	15.3	29.1	20	18.1	31.4	23.9	20.9	18.9	18.9	16.3
5,6-Diisoprop.-3-Met. Phen.	± 12.70	40.7	103.9	83	63.8	105.9	79.9	72.9	68.5	51.5	53.1
Heavies	± 13.04	66.6	62.1	50.2	21	41.6	32.2	26	20.7	17.7	16.3
Heavies		49.8	67.9	69	54.6	70.4	47.9	54.3	38.6	36.2	39.5

Table 0.11: GC raw data for simulated washcoating (cont.)

		WC-11	WC-12	WC-13	WC-14	WC-15	WC-16	WC-17	WC-18	WC-19	WC-20
Time on Stream		37:00:44	42:54:44	55:00:44	62:00:44	64:00:44	66:00:44	76:00:44	78:00:44	80:00:44	82:00:44
Entry Temperature		101	103	100	102	105	105	99	102	101	101
Temperature		275	275	275	276	275	275	275	275	275	275
WHSV		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	123.2	45	36.1	33.9	56.5	40.9	41.1	29.8	44.2	39
???	± 5.04	3.5	1.1			1					
phenol	± 5.26	22.1	8	5.5	4.9	8.6	4.9	5.7	4	5.7	5.2
o-Cresol	± 5.35	28.9	7.8	5.4	5.6	11.8	6.6	7.2	4.7	7.7	6.8
p-Cresol	± 5.60	227.9	80.6	57.7	52.9	100.7	58.4	67	44.3	72.6	67.1
m-Cresol	± 5.80	35165.7	12646.4	9107.1	8259.2	16067.5	9138.5	10731.5	7003.7	11554.3	10650.4
???	± 6.00	36.3	13.1	10.1	9.3	11.1	6.3	7.9	5.4	7.1	7.3
2,4-Xylenol	± 6.20	15.4	3.9	2.6	2.3	4.7	2.8	3.4	2.9	3.3	3.1
2,5-Xylenol	± 6.50	25.2	8.8	7.3	4.1	10.3	4.9	4.9	4.5	4.6	7.4
2,3-Xylenol	± 6.74	13.2	5.5	2.4	4.3	3.4	3	4	2.6	3.6	4
???	± 6.90	7.7	2.4	1.6	1.8	2.1	1.4	1.5	2	2.1	2.8
???	± 7.03	1.9									
???	± 7.16	11.6	4	2	1.9	3.2	2	2	1.1	2.1	1.8
2-Isopropyl-4-methyl Phenol	± 7.30	116	46.3	30.3	25.8	46.9	27.2	29.4	20.6	31.2	31.5
???	± 7.49	12.1	4.9	2.5	1.9	3.3	2	2.2	1.4	2.1	1.5
Thymol isomer (2,3)	± 7.60	1600.9	640.8	462.1	420.3	764.8	484.4	534.3	381.4	593.2	554.1
???	± 7.73	18.9	7.7	4	2.9	5.4	3.1	3	2.3	2.9	2.6
Thymol	± 7.90	13099.4	5029	3089.4	2685.7	4859.5	2730.1	2892.2	2001	3042.9	2834.6
????	± 8.19	31.3	10.8	5.9	4.6	8.4	4.2	4.2	3.3	4.7	4.3
????	± 8.33	198.7	73.9	38.2	31.3	54.7	27.6	28.5	19.1	28.2	25.5
6-n-Propyl-3-Methyl Phenol	± 8.40	440.7	180.1	112	104.6	161.5	112.1	103.7	76	109.2	100.6
2,6-Diisoprop.-3-Met. Phen.	± 8.55	17	6.6	2.3	2	4.9	3.8	2.3	1.5	2.4	2.2
5,3 Thymol isomer	± 8.67	713.6	282.9	154.7	130.5	222.9	130.4	111.2	146.3	131.3	123
4,3 Thymol isomer	± 8.78	2237.3	921.6	553.1	506.1	848.5	513.8	531.7	508.5	558.3	525.8
C-13 fraction (13.02)	± 8.83	2.4	1	1.1	1.1	0.7	0.6	0.5	1.2	1.8	1.1
????	± 9.22	22	8.2	4.8	3.2	5.8	3.4	3.9	1.8	3	4.1
????	± 9.48	28.1	10.6	4.9	5.1	7.1	3.8	4.1	3.4	4.5	5.2
????	± 9.60	5.8	2.9	1	1.8	1.5	1.4	0.6	1.1	1.6	1.2
????	± 10.30	10.9	2.6	2.2	2	2.2	0.5	1	0.4	1.1	1.4
????	± 10.70	7.2	3.4	3.2	2.6	2.8	1.8	1.6	1.9	2	1.9
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1422.6	601.8	323.8	316.3	449.5	314.2	267.3	193.9	292.2	268.4
????	± 11.30										
????	± 11.80										
????	± 12.09										
????	± 12.21	32.7	13.9	7.5	6.7	9.5	8.1	6.2	3.8	6.2	4.8
5,6-Diisoprop.-3-Met. Phen.	± 12.70	108	47.2	25.4	26.6	35.5	26.3	21.9	14.7	24.6	23.4
Heavies	± 13.04	33.8	12.5	6	7.1	8.5	5.4	4.8	3.8	5.6	5.1
Heavies		32.1	30.7	30.7	26.4	28.1	24.3	23.2	21.3	23.3	27.2

Table 0.12: GC raw data for simulated washcoating (cont.)

		WC-21	WC-22	WC-23	WC-24	WC-25	WC-26	WC-27	WC-28	WC-29	WC-30	WC-31	WC-32
Time on Stream		84:00:44	85:50:44	101:00:44	102:00:44	103:00:11	104:01:34	113:00:34	127:59:34	129:01:34	130:01:34	131:01:34	131:47:34
Entry Temperature		100	102	101	101	101	105	88	89	90	90	90	90
Temperature		275	275	275	275	275	275	275	275	275	275	274	275
WHSV		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.2	1.2	1.2	1.2	1.2
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.15	0.15	0.15	0.15
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	39.4	32.3	62.6	43.1	39.6	61.5	40.6	47	43.3	51.5	31.6	46.7
???	± 5.04												
phenol	± 5.26	4.9	4	5.6	3.4	3.9	5.2	5.1	4.3	3.7	4.2	2.8	2.9
o-Cresol	± 5.35	6.8	5.2	10.1	6.4	6.4	20.5	9.8	10	6.6	10.3	5	8.1
p-Cresol	± 5.60	64.4	49.7	90.3	61.9	58.3	95.1	87.1	76.7	64.7	79.3	47.7	72.9
m-Cresol	± 5.80	10336.5	7935.1	14502.6	9913.8	9335.7	19239.2	14216.1	12214.5	10445.2	12640.6	7609.4	11991.6
???	± 6.00	7.6		9.7	6.8	6.9	11.1	16.8	8.6	2.3	2.9	5	8.3
2,4-Xylenol	± 6.20	2.8	1.5	3.2	2.2	1.3	3.2	2.8	2.6	6	6.8	1.8	3.6
2,5-Xylenol	± 6.50	6.7	4.7	5.2	5	5	7.9	8.4	6.6	1.5	2.3	4.5	5.9
2,3-Xylenol	± 6.74	2.4	1.7	1.3	2.1	1.4	2.4	1.9	1.8	1.8	2	1.3	1.8
???	± 6.90	1.2											
???	± 7.03												
???	± 7.16	1.8	1.9	1.5	1.3	0.9	1.6	1.9	2.3	1.1	1.3	0.8	1.3
2-Isopropyl-4-methyl Phenol	± 7.30	26.8	21.3	33.4	23.7	21.5	33.8	33.5	71	23.9	28.9	16.9	26.2
???	± 7.49	1.6	1.5				2.4	1.7	1.3	0.9	1	0.6	
Thymol isomer (2,3)	± 7.60	522.5	404.7	734.1	525.4	459.9	774	695.5	694.2	584.5	714.8	418.2	664.4
???	± 7.73	2.6	2.2										
Thymol	± 7.90	2618.6	2028.4	3098.6	2170.2	1922.7	3183.1	3084.5	2506.6	2058.3	2545.8	1458.1	2322.7
????	± 8.19	4	3.2					3.5					
????	± 8.33	23.7	18.2	23.7	16.5	14.9	23.2	21.7	18.5	11	14.3	7.3	12.5
6-n-Propyl-3-Methyl Phenol	± 8.40	93.9	75.4	109	80.8	71.8	115.3	102.6	98.2	81	100.1	55.4	107.2
2,6-Diisoprop.-3-Met. Phen.	± 8.55	1.7	1.5										
5,3 Thymol isomer	± 8.67	112.1	87.4	124.2	86.2	77.4	124.3	113.5	88.9	72.7	88.5	50.2	81.4
4,3 Thymol isomer	± 8.78	481.2	374.1	561.6	399	356.1	576.5	509.5	454	362.6	467.1	267.4	424.9
C-13 fraction (13.02)	± 8.83	1.3	1.1	1.4	0.8	0.9	1.2	1					
????	± 9.22	2.5	2	3.7	2.1	1.9	3	2.3	1.1	1.3	1.4	10.9	1
????	± 9.48	3.2	2.8	3.8	2.8	2.2	4.4	3.4	2.8	3.2	2	1.5	2.9
????	± 9.60	0.9	1.8										
????	± 10.30	1.2	1.9										
????	± 10.70	1.6	1.8						5.4				
4,6-Diisoprop.-3-Met. Phen.	± 11.18	244.8	193.4	255.4	186.8	170.7	257.6	235.4	211.1	162.6	213.1	120.5	193.6
????	± 11.30												
????	± 11.80												
????	± 12.09												
????	± 12.21	5.6	5	5.4	4.6	5	6.2	5.4	4.6	4	6.4	4.1	4.8
5,6-Diisoprop.-3-Met. Phen.	± 12.70	20.1	16.7	21.5	15.8	13.5	21.5	18.3	17.4	15.3	17.3	10.7	15.3
Heavies	± 13.04	4.4	2.9	4.8	3.9	3	4	3.6	4.2	2.8	2.3	1.8	2
Heavies		26.3	24.2	15.6	19.1	18.3	28.6	19.3	28.3	21.5	22.1	21.7	11.5

Table 0.13: GC raw data for simulated washcoating (cont.)

		WC-33	WC-34	WC-35	WC-36	WC-37	WC-38	WC-39	WC-40	WC-41	WC-42	WC-43
Time on Stream		172:01:34	174:01:34	176:01:34	178:01:34	179:57:34	183:55:37	193:01:37	194:01:37	195:01:37	196:01:37	196:59:37
Entry Temperature		92	93	94	94	94	93	90	91	91	89	88
Temperature		274	274	274	274	275	276	275	275	275	275	275
WHSV		0.3	0.3	0.3	0.3	0.3	0.3	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.037	0.037	0.037	0.037	0.037	0.037	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	36	22.3	14.1	34.1	33.3	18.4	78.1	44.5	45.8	39.8	590
???	± 5.04											8
phenol	± 5.26	5.9	3.8	2.8	5.2	5.4		5.9	3.5	3.9	3.2	39.7
o-Cresol	± 5.35	9.9	4.8	1.4	8.5	8.7	3.4	13.5	6	7.2	6.5	109.5
p-Cresol	± 5.60	71.5	40.6	24.1	67.8	68.4	33.7	124.1	61.4	76.2	64.3	858.1
m-Cresol	± 5.80	11701.5	6662.3	3822.5	11046.8	11314.3	5377.2	19998.8	9848	12294.6	10269.3	134328.7
???	± 6.00	8.5	10	3.2	13	7.9	3.9	14.6	6.5	7.4	7.2	95.4
2,4-Xylenol	± 6.20	8	15.2	4.2	14.8	6.9	2.8	7.2	2.5	3.1	5.6	52.2
2,5-Xylenol	± 6.50	0.8	3.2	2.6		13.1	1.9	10.9	5.5	5.3		8.2
2,3-Xylenol	± 6.74	14	3.2	3.5	3.7	3.5	1.7	3.4	1.1	1.9	1.9	16.8
???	± 6.90	4.8	1.9	1.4	1.3	1.6	2.2					6.4
???	± 7.03											
???	± 7.16	5.3	3.4	2.2	4.4	4.7	4.3	2.1	0.8	1.1	1	9.5
2-Isopropyl-4-methyl Phenol	± 7.30	68.3	45.5	28.8	61.3	62.3	28.5	44	21.1	25.1	21.4	227.8
???	± 7.49	9.2	6.4	3.9	9.3	8.1	3.9	1.8	1.5	1.2	3.5	7
Thymol isomer (2,3)	± 7.60	560.5	354.3	201.7	489.3	496.1	246.4	1107.2	527.4	643.6	556.5	6586.4
???	± 7.73											
Thymol	± 7.90	7224.1	4715.6	2950	6512.5	6491.8	2847.7	4036.3	1815.5	2232.3	1882.6	20769.3
????	± 8.19											20
????	± 8.33	61.2	39.1	24.6	53.5	52.2	24.1	20.1	8.4	2	6.4	92.3
6-n-Propyl-3-Methyl Phenol	± 8.40	252.2	172.4	119	241.6	216.7	105.1	168.5	70.1	99.1	72.8	718.9
2,6-Diisoprop.-3-Met. Phen.	± 8.55				3.3							
5,3 Thymol isomer	± 8.67	544.8	338.2	221.2	483.9	450.1	231.1	156.2	66.1	80.3	68.2	657.2
4,3 Thymol isomer	± 8.78	1058.5	672.2	426.4	992.4	946.8	417.1	772.6	337.3	411.7	361.5	3706.4
C-13 fraction (13.02)	± 8.83	1.6	1.3	1.3	2.1	1.7	2.2					
????	± 9.22	16.2	10.7	7.3	15.3	13.6	6.2	2	0.9	2.1	1	10.8
????	± 9.48	11.8	7.2	3.8	11.9	10	5	3.9	2.7	1.8	2.2	16.4
????	± 9.60	5.2	3.7	2.7	3.9	3.9	2.2	3.3	1.1	1.4	1.6	3.8
????	± 10.30	9.4	3.5	1.4	3.1	3.4	3.3	1				2.2
????	± 10.70	5.9	3.4	2.2	5.6	3.9	2.2	3.4				4.7
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1256.6	818.1	577.9	1273.4	1055.7	502.9	371.7	163.9	183.7	158.9	1446.2
????	± 11.30							4.8				
????	± 11.80											
????	± 12.09											
????	± 12.21	23.7	15.8	10.5	23.3	19.5	8.8	10	4.4	4.7	4.2	34.4
5,6-Diisoprop.-3-Met. Phen.	± 12.70	70.7	45.1	33.7	71.3	58.3	30.3	31.6	12.8	15.5	14.1	127.5
Heavies	± 13.04	38.3	24.5	18.7	37.7	31.1	14	5.7	2.3	2.2	2.2	22.7
Heavies		16.9	18.2	14.3	21.3	20	16.5	15.3	12.6	14.2	18.7	18.7

Table 0.14: GC raw data for simulated washcoating (cont.)

		WC-44	WC-45	WC-46	WC-47	WC-48	WC-49	WC-50	WC-51	WC-52	WC-53	WC-54	WC-55
Time on Stream		201:01:37	202:01:37	203:01:37	204:01:37	206:01:37	207:01:37	207:31:37	208:01:37	208:31:12	217:01:12	218:01:12	219:01:12
Entry Temperature		88	89	89	88	84	83	83	83	83	90	91	91
Temperature		275	275	275	275	274	274	275	275	275	275	275	274
WHSV		1.81	181	1.81	1.81	3.63	3.63	3.63	3.63	3.63	1.28	1.28	1.28
Pump Rate (ml/min)		0.227	0.227	0.227	0.227	0.454	0.454	0.454	0.454	0.454	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	59.7	83.7	61.2	162.6	297.2	244	252.8	229	222.5	309	222.6	254.9
???	± 5.04				1.4								
phenol	± 5.26	2	2.7	1.5	3.3								
o-Cresol	± 5.35	6.7	9	4.8	14.6	8.8	6.1	6.9	6.1	6.8	5.9	4.5	4.5
p-Cresol	± 5.60	65.6	86.7	46.4	129.7	82.2	56.1	58.8	54.4	58.3	57.5	41.5	45.1
m-Cresol	± 5.80	10586.6	14026.8	7425.5	20983.7	13379.8	9072	9519.7	8795.3	9502.2	9347.1	6656.3	7297.5
???	± 6.00	7.1	9.7	4.3	23.9	9.1	6.4	6.4	5.3	6.5	7.2	4.5	5.6
2,4-Xylenol	± 6.20	1.4	2.3	1.1	9.2	1.4	2.8	1.6	0.7	3.6	3.5	1	3
2,5-Xylenol	± 6.50	4	5.1	2.5		4.6	3.4	3.3	3.2	3.1	2.3	2.6	2.4
2,3-Xylenol	± 6.74				2.3	2.8	1.6	1.6	1.2	1.4	2.1	2	2.2
???	± 6.90												
???	± 7.03												
???	± 7.16												
2-Isopropyl-4-methyl Phenol	± 7.30	15	20.5	9.5	26.9	8.3	5.4	5.9	4.9	6.7	10	7.3	8.7
???	± 7.49												
Thymol isomer (2,3)	± 7.60	504	633.3	329.7	950.5	361	231.9	263.4	217.2	267.6	420.6	298.1	343.8
???	± 7.73												
Thymol	± 7.90	1175.3	1439.9	715.6	2003.2	598.9	362.8	404.5	326.7	401.4	701.1	499.6	583.8
????	± 8.19												
????	± 8.33	4	4.8	2.1	6.6								
6-n-Propyl-3-Methyl Phenol	± 8.40	39	45.6	23.7	58.1	12.6	7.4	9.1	6.7	9.2	31.2	14.7	17.7
2,6-Diisoprop.-3-Met. Phen.	± 8.55												
5,3 Thymol isomer	± 8.67	37.7	43.8	21.8	55.8	17.7	8.3	8.9	6.6	9	13.8	11.3	13.1
4,3 Thymol isomer	± 8.78	240.3	292	136.8	391.8	132.5	67.5	71.2	52.9	66.5	109.6	82.6	94.8
C-13 fraction (13.02)	± 8.83												
????	± 9.22												
????	± 9.48												
????	± 9.60												
????	± 10.30												
????	± 10.70												
4,6-Diisoprop.-3-Met. Phen.	± 11.18	78.3	91	44.6	109	27.6	14.6	16	12.3	13.6	37.1	27.5	34.1
????	± 11.30												
????	± 11.80												
????	± 12.09												
????	± 12.21	2.1											
5,6-Diisoprop.-3-Met. Phen.	± 12.70	10	9.7	6.4	13.7	6.2	3.1	3.9	3.4	2.4	5.8	3.7	5.6
Heavies	± 13.04												
Heavies		19.9	22.4	22.2	23.2	21.3	20.1	23.8	22.3	25.2	21.8	23.8	22.5

Table 0.15: Product composition (%) for simulated washcoating

		WC-1	WC-2	WC-3	WC-4	WC-5	WC-6	WC-7	WC-8	WC-9	WC-10
Time on Stream		07:10:44	08:10:44	09:00:44	11:00:44	11:50:44	14:30:44	17:30:44	31:40:44	33:00:44	35:00:44
Entry Temperature		103	103	104	105	105	105	105	101	104	103
Temperature		274	277	278	276	275	275	275	275	275	275
WHSV		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.02	0.10	0.10	0.11	0.12	0.12	0.13	0.14	0.16	0.17
???	± 5.04	0.06	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
phenol	± 5.26	0.01	0.02	0.02	0.02	0.02	-	0.02	0.03	0.03	0.03
o-Cresol	± 5.35	0.41	0.07	0.05	0.05	0.05	0.05	0.05	0.05	0.06	0.06
p-Cresol	± 5.60	1.84	0.44	0.41	0.38	0.40	0.41	0.41	0.44	0.45	0.45
m-Cresol	± 5.80	75.38	56.09	53.90	53.87	56.37	58.88	60.21	65.30	67.45	68.31
???	± 6.00	0.04	0.06	0.08	0.04	0.03	0.06	0.06	0.10	0.06	0.04
2,4-Xylenol	± 6.20	0.08	0.06	0.08	0.04	0.04	0.03	0.03	0.05	0.03	0.02
2,5-Xylenol	± 6.50	0.05	0.04	0.07	0.04	0.05	0.05	0.03	0.06	0.04	0.03
2,3-Xylenol	± 6.74	0.05	0.05	0.03	0.03	0.03	0.03	0.04	0.03	0.02	0.01
???	± 6.90	0.06	0.03	0.03	0.02	0.02	0.02	0.03	0.02	0.02	0.02
???	± 7.03	0.02	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.02
???	± 7.16	0.11	0.07	0.06	0.04	0.05	0.04	0.03	0.02	0.02	0.02
2-Isopropyl-4-methyl Phenol	± 7.30	0.16	0.27	0.28	0.23	0.25	0.24	0.24	0.21	0.20	0.20
???	± 7.49	0.06	0.07	0.06	0.04	0.05	0.04	0.04	0.04	0.03	0.02
Thymol isomer (2,3)	± 7.60	0.47	1.37	1.47	1.57	1.81	1.84	1.98	2.10	2.11	2.26
???	± 7.73	0.18	0.11	0.11	7.35	0.07	0.07	0.06	0.10	0.04	0.03
Thymol	± 7.90	12.68	27.56	29.22	24.82	27.45	26.33	25.20	21.93	20.65	20.01
????	± 8.19	0.15	0.13	0.13	0.09	0.10	0.09	0.08	0.06	0.06	0.05
????	± 8.33	1.60	1.09	1.14	0.79	0.81	0.73	0.62	0.44	0.39	0.35
6-n-Propyl-3-Methyl Phenol	± 8.40	0.18	0.65	0.71	0.71	0.85	0.76	0.80	0.75	0.70	0.68
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.08	0.10	0.10	0.07	0.07	0.06	0.05	0.04	0.03	0.02
5,3 Thymol isomer	± 8.67	1.93	2.68	2.69	1.99	2.24	2.04	1.86	1.42	1.27	1.24
4,3 Thymol isomer	± 8.78	2.04	4.48	4.69	4.14	4.80	4.51	4.48	4.00	3.69	3.60
C-13 fraction (13.02)	± 8.83	0.03	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00
????	± 9.22	0.27	0.19	0.17	0.10	0.11	0.08	0.07	0.04	0.03	0.04
????	± 9.48	0.14	0.10	0.10	0.07	0.08	0.07	0.06	0.04	0.04	0.04
????	± 9.60	0.04	0.03	0.03	0.02	0.02	0.02	0.02	0.03	0.01	0.01
????	± 10.30	0.08	0.13	0.11	0.07	0.07	0.06	0.05	0.02	0.02	0.02
????	± 10.70	0.31	0.03	0.02	0.01	0.02	0.02	0.02	0.03	0.01	0.01
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1.22	3.31	3.39	2.74	3.40	2.86	2.80	2.09	2.02	1.88
????	± 11.30	0.02	-	-	-	-	-	-	0.02	-	-
????	± 11.80	0.01	0.00	-	-	-	-	-	-	-	-
????	± 12.09	0.02	0.01	-	-	-	-	-	-	-	-
????	± 12.21	0.05	0.07	0.07	0.06	0.08	0.06	0.06	0.05	0.06	0.04
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.12	0.24	0.27	0.21	0.26	0.21	0.21	0.16	0.15	0.15
Heavies	± 13.04	0.20	0.15	0.16	0.07	0.10	0.08	0.07	0.05	0.05	0.04
Heavies		0.15	0.16	0.23	0.18	0.17	0.13	0.16	0.09	0.11	0.11

Table 0.16: Product composition (%) for simulated washcoating (cont.)

		WC-11	WC-12	WC-13	WC-14	WC-15	WC-16	WC-17	WC-18	WC-19	WC-20
Time on Stream		37:00:44	42:54:44	55:00:44	62:00:44	64:00:44	66:00:44	76:00:44	78:00:44	80:00:44	82:00:44
Entry Temperature		101	103	100	102	105	105	99	102	101	101
Temperature		275	275	275	276	275	275	275	275	275	275
WHSV		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.18	0.18	0.21	0.22	0.19	0.24	0.21	0.23	0.21	0.20
???	± 5.04	0.01	0.01	-	-	0.00	-	-	-	-	-
phenol	± 5.26	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
o-Cresol	± 5.35	0.06	0.04	0.04	0.05	0.06	0.05	0.05	0.05	0.05	0.05
p-Cresol	± 5.60	0.46	0.44	0.46	0.47	0.47	0.48	0.48	0.48	0.48	0.48
m-Cresol	± 5.80	71.49	69.75	72.90	73.35	75.32	74.74	76.94	75.53	77.17	76.94
???	± 6.00	0.06	0.06	0.06	0.06	0.04	0.04	0.04	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
2,5-Xylenol	± 6.50	0.04	0.04	0.04	0.03	0.04	0.03	0.03	0.04	0.02	0.04
2,3-Xylenol	± 6.74	0.02	0.02	0.01	0.03	0.01	0.02	0.02	0.02	0.02	0.02
???	± 6.90	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.02
???	± 7.03	0.00	-	-	-	-	-	-	-	-	-
???	± 7.16	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.18	0.20	0.19	0.18	0.17	0.17	0.16	0.17	0.16	0.17
???	± 7.49	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Thymol isomer (2,3)	± 7.60	2.23	2.42	2.54	2.56	2.46	2.72	2.63	2.82	2.72	2.75
???	± 7.73	0.03	0.03	0.02	0.02	0.02	0.02	0.01	0.02	0.01	0.01
Thymol	± 7.90	18.26	19.02	16.96	16.36	15.62	15.31	14.22	14.80	13.94	14.04
????	± 8.19	0.04	0.04	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02
????	± 8.33	0.28	0.28	0.21	0.19	0.18	0.15	0.14	0.14	0.13	0.13
6-n-Propyl-3-Methyl Phenol	± 8.40	0.61	0.68	0.61	0.64	0.52	0.63	0.51	0.56	0.50	0.50
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.02	0.02	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01
5,3 Thymol isomer	± 8.67	0.99	1.07	0.85	0.79	0.72	0.73	0.72	0.68	0.60	0.61
4,3 Thymol isomer	± 8.78	3.12	3.49	3.04	3.08	2.73	2.88	3.12	2.84	2.56	2.61
C-13 fraction (13.02)	± 8.83	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.00
????	± 9.22	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.02
????	± 9.48	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
????	± 9.60	0.01	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.01	0.00
????	± 10.30	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.01
????	± 10.70	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1.51	1.73	1.35	1.47	1.10	1.34	1.00	1.09	1.02	1.01
????	± 11.30	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.03	0.04	0.03	0.03	0.02	0.03	0.02	0.02	0.02	0.02
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.11	0.14	0.11	0.12	0.09	0.11	0.08	0.08	0.09	0.09
Heavies	± 13.04	0.04	0.04	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02
Heavies		0.03	0.09	0.13	0.12	0.07	0.10	0.09	0.12	0.08	0.10

Table 0.17: Product composition (%) for simulated washcoating (cont.)

		WC-21	WC-22	WC-23	WC-24	WC-25	WC-26	WC-27	WC-28	WC-29	WC-30	WC-31	WC-32
Time on Stream		84:00:44	85:50:44	101:00:44	102:00:44	103:00:11	104:01:34	113:00:34	127:59:34	129:01:34	130:01:34	131:01:34	131:47:34
Entry Temperature		100	102	101	101	101	105	88	89	90	90	90	90
Temperature		275	275	275	275	275	275	275	275	275	275	274	275
$WHSV_{Wet}$		1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.2	1.2	1.2	1.2	1.2
Pump Rate (mL/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.15	0.15	0.15	0.15
Guage Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.21	0.23	0.25	0.25	0.25	0.19	0.17	0.22	0.24	0.24	0.24	0.23
???	± 5.04	-	-	-	-	-	-	-	-	-	-	-	-
phenol	± 5.26	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
o-Cresol	± 5.35	0.05	0.05	0.06	0.05	0.06	0.09	0.06	0.07	0.05	0.07	0.05	0.05
p-Cresol	± 5.60	0.48	0.49	0.50	0.50	0.50	0.42	0.49	0.50	0.50	0.51	0.51	0.49
m-Cresol	± 5.80	77.78	77.59	80.36	79.83	80.73	83.99	80.52	80.35	81.20	80.83	81.40	81.35
???	± 6.00	0.04	-	0.04	0.04	0.05	0.04	0.07	0.04	0.01	0.01	0.04	0.04
2,4-Xylenol	± 6.20	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.04	0.03	0.01	0.02
2,5-Xylenol	± 6.50	0.04	0.04	0.02	0.03	0.03	0.03	0.04	0.03	0.01	0.01	0.04	0.03
2,3-Xylenol	± 6.74	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
???	± 6.90	0.01	-	-	-	-	-	-	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.15	0.16	0.14	0.15	0.14	0.11	0.15	0.36	0.14	0.14	0.14	0.14
???	± 7.49	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00	-
Thymol isomer (2,3)	± 7.60	2.70	2.71	2.79	2.90	2.73	2.32	2.70	3.13	3.12	3.13	3.07	3.09
???	± 7.73	0.01	0.01	-	-	-	-	-	-	-	-	-	-
Thymol	± 7.90	13.52	13.60	11.78	11.99	11.40	9.53	11.98	11.31	10.97	11.16	10.70	10.81
????	± 8.19	0.02	0.02	-	-	-	-	0.01	-	-	-	-	-
????	± 8.33	0.12	0.12	0.09	0.09	0.09	0.07	0.08	0.08	0.06	0.06	0.05	0.06
6-n-Propyl-3-Methyl Phenol	± 8.40	0.48	0.51	0.41	0.45	0.43	0.35	0.40	0.44	0.43	0.44	0.41	0.50
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.01	0.01	-	-	-	-	-	-	-	-	-	-
5,3 Thymol isomer	± 8.67	0.58	0.59	0.47	0.48	0.46	0.37	0.44	0.40	0.39	0.39	0.37	0.38
4,3 Thymol isomer	± 8.78	2.48	2.51	2.13	2.20	2.11	1.73	1.98	2.05	1.93	2.05	1.96	1.98
C-13 fraction (13.02)	± 8.83	0.01	0.01	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-
????	± 9.22	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.06	0.00
????	± 9.48	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
????	± 9.60	0.00	0.01	-	-	-	-	-	-	-	-	-	-
????	± 10.30	0.00	0.01	-	-	-	-	-	-	-	-	-	-
????	± 10.70	0.01	0.01	-	-	-	-	-	0.02	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.96	0.99	0.74	0.79	0.77	0.59	0.70	0.72	0.66	0.71	0.67	0.69
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.02	0.03	0.02	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.08	0.09	0.06	0.07	0.06	0.05	0.05	0.06	0.06	0.06	0.06	0.05
Heavies	± 13.04	0.02	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Heavies		0.10	0.12	0.05	0.08	0.08	0.07	0.06	0.10	0.09	0.07	0.12	0.04

Table 0.18: Product composition (%) for simulated washcoating (cont.)

		WC-33	WC-34	WC-35	WC-36	WC-37	WC-38	WC-39	WC-40	WC-41	WC-42	WC-43
Time on Stream		172:01:34	174:01:34	176:01:34	178:01:34	179:57:34	183:55:37	193:01:37	194:01:37	195:01:37	196:01:37	196:59:37
Entry Temperature		92	93	94	94	94	93	90	91	91	89	88
Temperature		274	274	274	274	275	276	275	275	275	275	275
WHSV		0.3	0.3	0.3	0.3	0.3	0.3	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)		0.037	0.037	0.037	0.037	0.037	0.037	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.13	0.14	0.15	0.14	0.13	0.16	0.23	0.27	0.22	0.23	0.27
???	± 5.04	-	-	-	-	-	-	-	-	-	-	0.01
phenol	± 5.26	0.02	0.02	0.03	0.02	0.02	-	0.02	0.02	0.02	0.02	0.02
o-Cresol	± 5.35	0.05	0.04	0.02	0.05	0.05	0.04	0.05	0.05	0.05	0.05	0.07
p-Cresol	± 5.60	0.37	0.35	0.35	0.38	0.38	0.40	0.50	0.51	0.51	0.51	0.54
m-Cresol	± 5.80	60.57	57.40	54.97	61.30	62.60	63.78	80.67	81.92	82.27	81.98	84.33
???	± 6.00	0.03	0.07	0.04	0.06	0.03	0.04	0.05	0.04	0.04	0.04	0.05
2,4-Xylenol	± 6.20	0.03	0.10	0.05	0.06	0.03	0.03	0.02	0.02	0.02	0.03	0.03
2,5-Xylenol	± 6.50	0.00	0.02	0.03	0.04	0.06	0.02	0.03	0.04	0.03	-	0.00
2,3-Xylenol	± 6.74	0.06	0.02	0.04	0.02	0.01	0.02	0.01	0.01	0.01	0.01	0.01
???	± 6.90	0.02	0.01	0.02	0.01	0.01	0.02	-	-	-	-	0.00
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.02	0.02	0.02	0.02	0.02	0.04	0.01	0.01	0.01	0.01	0.00
2-Isopropyl-4-methyl Phenol	± 7.30	0.27	0.30	0.32	0.26	0.26	0.26	0.14	0.13	0.13	0.13	0.11
???	± 7.49	0.04	0.04	0.04	0.04	0.03	0.04	0.01	0.01	0.01	0.01	0.00
Thymol isomer (2,3)	± 7.60	1.99	2.09	1.99	1.86	1.88	2.00	3.06	3.01	2.95	3.05	2.84
???	± 7.73	-	-	-	-	-	-	-	-	-	-	-
Thymol	± 7.90	25.65	27.87	29.09	24.79	24.63	23.17	11.17	10.36	10.24	10.31	8.94
????	± 8.19	-	-	-	-	-	-	-	-	-	-	0.01
????	± 8.33	0.22	0.23	0.24	0.20	0.20	0.20	0.06	0.05	0.01	0.04	0.04
6-n-Propyl-3-Methyl Phenol	± 8.40	0.90	1.02	1.17	0.92	0.82	0.86	0.47	0.40	0.45	0.40	0.31
2,6-Diisoprop.-3-Met. Phen.	± 8.55	-	-	-	0.01	-	-	-	-	-	-	-
5,3 Thymol isomer	± 8.67	1.93	2.00	2.18	1.84	1.71	1.88	0.43	0.38	0.37	0.37	0.28
4,3 Thymol isomer	± 8.78	3.76	3.97	4.21	3.78	3.59	3.39	2.14	1.92	1.89	1.98	1.60
C-13 fraction (13.02)	± 8.83	0.00	0.01	0.01	0.01	0.00	0.01	-	-	-	-	-
????	± 9.22	0.04	0.05	0.05	0.04	0.04	0.04	0.00	0.00	0.01	0.00	0.00
????	± 9.48	0.03	0.03	0.03	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.01
????	± 9.60	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.00	-	0.01	0.00
????	± 10.30	0.03	0.02	0.01	0.01	0.01	0.02	0.00	-	-	-	0.00
????	± 10.70	0.02	0.02	0.02	0.02	0.01	0.01	0.01	-	-	-	0.00
4,6-Diisoprop.-3-Met. Phen.	± 11.18	3.39	3.68	4.34	3.69	3.05	3.11	0.78	0.71	0.64	0.66	0.47
????	± 11.30	-	-	-	-	-	-	0.01	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.06	0.07	0.08	0.07	0.06	0.05	0.02	0.02	0.02	0.02	0.01
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.19	0.20	0.25	0.21	0.17	0.19	0.07	0.06	0.05	0.06	0.04
Heavies	± 13.04	0.10	0.11	0.14	0.11	0.09	0.09	0.01	0.01	0.01	0.01	0.01
Heavies		0.05	0.08	0.11	0.06	0.06	0.10	0.03	0.05	0.05	0.08	0.01

Table 0.19: Product composition (%) for simulated washcoating (cont.)

		WC-44	WC-45	WC-46	WC-47	WC-48	WC-49	WC-50	WC-51	WC-52	WC-53	WC-54	WC-55
Time on Stream		201:01:37	202:01:37	203:01:37	204:01:37	206:01:37	207:01:37	207:31:37	208:01:37	208:31:12	217:01:12	218:01:12	219:01:12
Entry Temperature		88	89	89	88	84	83	83	83	83	90	91	91
Temperature		275	275	275	275	274	274	275	275	275	275	275	274
WHSV		1.81	181	1.81	1.81	3.63	3.63	3.63	3.63	3.63	1.28	1.28	1.28
Pump Rate (ml/min)		0.227	0.227	0.227	0.227	0.454	0.454	0.454	0.454	0.454	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.35	0.38	0.52	0.49	1.47	1.79	1.76	1.74	1.56	2.11	2.13	2.21
???	± 5.04	-	-	-	0.01	-	-	-	-	-	-	-	-
phenol	± 5.26	0.01	0.01	0.01	0.01	-	-	-	-	-	-	-	-
o-Cresol	± 5.35	0.06	0.06	0.06	0.06	0.06	0.06	0.07	0.06	0.07	0.06	0.06	0.05
p-Cresol	± 5.60	0.54	0.54	0.55	0.55	0.57	0.57	0.57	0.57	0.57	0.54	0.55	0.54
m-Cresol	± 5.80	87.10	87.86	88.22	88.35	92.25	92.48	92.21	92.87	92.41	88.50	88.44	87.90
???	± 6.00	0.04	0.05	0.04	0.08	0.05	0.05	0.05	0.04	0.05	0.05	0.05	0.05
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.03	0.01	0.02	0.01	0.01	0.03	0.03	0.01	0.03
2,5-Xylenol	± 6.50	0.03	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.03	0.02
2,3-Xylenol	± 6.74	-	-	-	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02
???	± 6.90	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	-	-	-	-	-	-	-	-	-	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	0.09	0.10	0.09	0.09	0.04	0.04	0.04	0.04	0.05	0.07	0.07	0.08
???	± 7.49	-	-	-	-	-	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	2.84	2.72	2.69	2.74	1.71	1.62	1.75	1.57	1.78	2.73	2.72	2.84
???	± 7.73	-	-	-	-	-	-	-	-	-	-	-	-
Thymol	± 7.90	6.63	6.19	5.83	5.78	2.83	2.54	2.69	2.37	2.68	4.55	4.55	4.82
????	± 8.19	-	-	-	-	-	-	-	-	-	-	-	-
????	± 8.33	0.02	0.02	0.02	0.02	-	-	-	-	-	-	-	-
6-n-Propyl-3-Methyl Phenol	± 8.40	0.22	0.20	0.19	0.17	0.06	0.05	0.06	0.05	0.06	0.20	0.13	0.15
2,6-Diisoprop.-3-Met. Phen.	± 8.55	-	-	-	-	-	-	-	-	-	-	-	-
5,3 Thymol isomer	± 8.67	0.21	0.19	0.18	0.16	0.08	0.06	0.06	0.05	0.06	0.09	0.10	0.11
4,3 Thymol isomer	± 8.78	1.36	1.25	1.11	1.13	0.63	0.47	0.47	0.38	0.44	0.71	0.75	0.78
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.22	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.48	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.60	-	-	-	-	-	-	-	-	-	-	-	-
????	± 10.30	-	-	-	-	-	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.34	0.30	0.28	0.24	0.10	0.08	0.08	0.07	0.07	0.18	0.19	0.21
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.01	-	-	-	-	-	-	-	-	-	-	-
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.04	0.03	0.04	0.03	0.02	0.02	0.02	0.02	0.01	0.03	0.03	0.04
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-	-	-
Heavies		0.09	0.07	0.14	0.05	0.08	0.11	0.12	0.12	0.13	0.11	0.17	0.14

Table 0.20: Conversion, selectivity and yield data for simulated washcoating

	WC-1	WC-2	WC-3	WC-4	WC-5	WC-6	WC-7	WC-8	WC-9	WC-10
Time on Stream	07:10:44	08:10:44	09:00:44	11:00:44	11:50:44	14:30:44	17:30:44	31:40:44	33:00:44	35:00:44
Entry Temperature	103	103	104	105	105	105	105	101	104	103
Temperature	274	277	278	276	275	275	275	275	275	275
$WHSV_{Wet}$	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guage Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	24.62	43.91	46.10	46.13	43.63	41.12	39.79	34.70	32.55	31.69
Thymol Selectivity	51.51	62.78	63.38	53.81	62.92	64.04	63.33	63.20	63.43	63.12
Thymol Yield	12.68	27.56	29.22	24.82	27.45	26.33	25.20	21.93	20.65	20.01
S3-isopropyl-5-methylphenol	**7.83**	**6.09**	**5.84**	**4.32**	**5.15**	**4.97**	**4.68**	**4.09**	**3.90**	**3.91**
Y3-methyl-5-isopropylphenol	1.93	2.68	2.69	1.99	2.24	2.04	1.86	1.42	1.27	1.24
S4-isopropyl-3-methylphenol	**8.30**	**10.21**	**10.18**	**8.97**	**10.99**	**10.96**	**11.26**	**11.52**	**11.33**	**11.36**
Y3-methyl-4-isopropylphenol	2.04	4.48	4.69	4.14	4.80	4.51	4.48	4.00	3.69	3.60
S2-isopropyl-3-methylphenol	**1.91**	**3.13**	**3.20**	**3.40**	**4.15**	**4.47**	**4.97**	**6.06**	**6.47**	**7.12**
Y3-methyl-2-isopropylphenol	0.47	1.37	1.47	1.57	1.81	1.84	1.98	2.10	2.11	2.26
Thymol	74.06	76.36	76.74	76.32	75.62	75.84	75.18	74.47	74.51	73.82
3-methyl-5-isopropylphenol	11.26	7.41	7.07	6.13	6.18	5.88	5.55	4.82	4.58	4.57
3-methyl-2-isopropylphenol	11.93	12.42	12.33	12.73	13.21	12.98	13.37	13.57	13.30	13.29
3-methyl-4-isopropylphenol	2.75	3.81	3.87	4.83	4.99	5.29	5.90	7.14	7.60	8.32
STotal.Isomer	**69.55**	**82.21**	**82.59**	**70.51**	**83.21**	**84.44**	**84.24**	**84.87**	**85.14**	**85.51**
YTotal.Isomer	17.13	36.10	38.07	32.53	36.30	34.72	33.52	29.45	27.71	27.10
Slights	2.20	1.52	1.53	1.07	1.18	1.25	1.28	1.55	1.28	1.22
Ylights	0.54	0.67	0.71	0.49	0.52	0.51	0.51	0.54	0.42	0.39
SC-10	7.25	3.03	2.98	17.83	2.26	2.17	1.93	1.73	1.48	1.38
YC-10	1.79	1.33	1.38	8.23	0.99	0.89	0.77	0.60	0.48	0.44
Sdi-isopropylated	6.28	8.66	8.50	6.68	8.76	7.80	7.86	6.76	6.93	6.61
Ydi-isopropylated	1.55	3.80	3.92	3.08	3.82	3.21	3.13	2.34	2.26	2.09
Sheavies	4.48	1.65	1.57	1.12	1.25	1.06	1.10	0.98	0.88	0.87
Yheavies	1.10	0.72	0.72	0.52	0.55	0.44	0.44	0.34	0.29	0.28
Sether	0.38	0.30	0.29	0.30	0.34	0.31	0.41	0.53	0.60	0.66
Yether	0.09	0.13	0.13	0.14	0.15	0.13	0.16	0.18	0.20	0.21

Table 0.21: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-11	WC-12	WC-13	WC-14	WC-15	WC-16	WC-17	WC-18	WC-19	WC-20
Time on Stream	37:00:44	42:54:44	55:00:44	62:00:44	64:00:44	66:00:44	76:00:44	78:00:44	80:00:44	82:00:44
Entry Temperature	101	103	100	102	105	105	99	102	101	101
Temperature	275	275	275	276	275	275	275	275	275	275
WHSV	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	28.51	30.25	27.10	26.65	24.68	25.26	23.06	24.47	22.83	23.06
Thymol Selectivity	64.05	62.89	62.60	61.39	63.29	60.62	61.69	60.48	61.06	60.90
Thymol Yield	18.26	19.02	16.96	16.36	15.62	15.31	14.22	14.80	13.94	14.04
S3-isopropyl-5-methylphenol	**3.49**	**3.54**	**3.13**	**2.98**	**2.90**	**2.90**	**13.79**	**14.63**	**2.63**	**2.64**
Y3-methyl-5-isopropylphenol	0.99	1.07	0.85	0.79	0.72	0.73	3.18	3.58	0.60	0.61
S4-isopropyl-3-methylphenol	**10.94**	**11.53**	**11.21**	**11.57**	**11.05**	**11.41**	**11.38**	**11.32**	**11.20**	**11.30**
Y3-methyl-4-isopropylphenol	3.12	3.49	3.04	3.08	2.73	2.88	2.76	2.67	2.56	2.61
S2-isopropyl-3-methylphenol	**7.83**	**8.01**	**9.36**	**9.61**	**9.96**	**10.76**	**11.40**	**11.53**	**11.90**	**11.91**
Y3-methyl-2-isopropylphenol	2.23	2.42	2.54	2.56	2.46	2.72	2.63	2.82	2.72	2.75
Thymol	74.21	73.16	72.53	71.76	72.58	70.75	71.01	69.81	70.34	70.21
3-methyl-5-isopropylphenol	4.04	4.12	3.63	3.49	3.33	3.38	3.28	3.19	3.04	3.05
3-methyl-2-isopropylphenol	12.68	13.41	12.99	13.52	12.67	13.32	13.39	13.12	12.91	13.02
3-methyl-4-isopropylphenol	9.07	9.32	10.85	11.23	11.42	12.55	13.12	13.31	13.71	13.72
STotal.Isomer	**86.31**	**85.97**	**86.31**	**85.56**	**87.21**	**85.68**	**86.88**	**86.64**	**86.81**	**86.75**
YTotal.Isomer	24.61	26.00	23.39	22.80	21.53	21.64	20.03	21.20	19.82	20.00
Slights	1.31	1.24	1.33	1.31	1.24	1.23	1.32	1.37	1.26	1.43
Ylights	0.37	0.38	0.36	0.35	0.31	0.31	0.30	0.33	0.29	0.33
SC-10	1.22	1.16	0.97	0.89	0.89	0.77	0.76	0.75	0.72	0.70
YC-10	0.35	0.35	0.26	0.24	0.22	0.20	0.18	0.18	0.16	0.16
Sdi-isopropylated	5.88	6.36	5.51	6.12	4.94	5.91	4.81	4.92	4.96	4.89
Ydi-isopropylated	1.68	1.92	1.49	1.63	1.22	1.49	1.11	1.20	1.13	1.13
Sheavies	0.53	0.70	0.85	0.85	0.57	0.74	0.67	0.80	0.66	0.77
Yheavies	0.15	0.21	0.23	0.23	0.14	0.19	0.15	0.20	0.15	0.18
Sether	0.77	0.72	0.88	0.93	0.91	1.07	1.05	1.07	1.05	1.00
Yether	0.22	0.22	0.24	0.25	0.22	0.27	0.24	0.26	0.24	0.23

Table 0.22: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-21	WC-22	WC-23	WC-24	WC-25	WC-26	WC-27	WC-28	WC-29	WC-30	WC-31	WC-32
Time on Stream	84:00:44	85:50:44	101:00:44	102:00:44	103:00:11	104:01:34	113:00:34	127:59:34	129:01:34	130:01:34	131:01:34	131:47:34
Entry Temperature	100	102	101	101	101	105	88	89	90	90	90	90
Temperature	275	275	275	275	275	275	275	275	275	275	274	275
WHSV	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.2	1.2	1.2	1.2	1.2
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.15	0.15	0.15	0.15
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	22.22	22.41	19.64	20.17	19.27	16.01	19.48	19.65	18.80	19.17	18.60	18.65
Thymol Selectivity	60.84	60.69	59.97	59.43	59.19	59.52	61.51	57.56	58.38	58.24	57.53	57.94
Thymol Yield	13.52	13.60	11.78	11.99	11.40	9.53	11.98	11.31	10.97	11.16	10.70	10.81
S3-isopropyl-5-methylphenol	**2.60**	**2.61**	**2.40**	**2.36**	**2.38**	**2.32**	**2.26**	**2.04**	**2.06**	**2.02**	**1.98**	**2.03**
Y3-methyl-5-isopropylphenol	0.58	0.59	0.47	0.48	0.46	0.37	0.44	0.40	0.39	0.39	0.37	0.38
S4-isopropyl-3-methylphenol	**11.18**	**11.19**	**10.87**	**10.93**	**10.96**	**10.78**	**10.16**	**10.42**	**10.28**	**10.69**	**10.55**	**10.60**
Y3-methyl-4-isopropylphenol	2.48	2.51	2.13	2.20	2.11	1.73	1.98	2.05	1.93	2.05	1.96	1.98
S2-isopropyl-3-methylphenol	**12.14**	**12.11**	**14.21**	**14.39**	**14.16**	**14.47**	**13.87**	**15.94**	**16.58**	**16.35**	**16.50**	**16.57**
Y3-methyl-2-isopropylphenol	2.70	2.71	2.79	2.90	2.73	2.32	2.70	3.13	3.12	3.13	3.07	3.09
Thymol	70.12	70.08	68.58	68.23	68.28	68.34	70.05	66.96	66.87	66.71	66.46	66.49
3-methyl-5-isopropylphenol	3.00	3.02	2.75	2.71	2.75	2.67	2.58	2.37	2.36	2.32	2.29	2.33
3-methyl-2-isopropylphenol	12.89	12.92	12.43	12.54	12.65	12.38	11.57	12.13	11.78	12.24	12.19	12.16
3-methyl-4-isopropylphenol	13.99	13.98	16.25	16.52	16.33	16.62	15.80	18.54	18.99	18.73	19.06	19.02
STotal.Isomer	**86.76**	**86.61**	**87.45**	**87.10**	**86.70**	**87.10**	**87.80**	**85.96**	**87.31**	**87.30**	**86.57**	**87.15**
YTotal.Isomer	19.27	19.41	17.17	17.57	16.70	13.95	17.10	16.89	16.41	16.74	16.10	16.25
Slights	1.32	1.09	1.17	1.26	1.27	1.30	1.49	2.42	1.19	1.15	1.36	1.31
Ylights	0.29	0.24	0.23	0.25	0.25	0.21	0.29	0.47	0.22	0.22	0.25	0.24
SC-10	0.70	0.71	0.46	0.45	0.46	0.43	0.50	0.42	0.31	0.33	0.29	0.31
YC-10	0.16	0.16	0.09	0.09	0.09	0.07	0.10	0.08	0.06	0.06	0.05	0.06
Sdi-isopropylated	4.79	4.88	4.15	4.30	4.39	4.03	3.90	4.07	3.90	4.05	3.99	4.00
Ydi-isopropylated	1.06	1.09	0.81	0.87	0.84	0.65	0.76	0.80	0.73	0.78	0.74	0.75
Sheavies	0.75	0.92	0.44	0.61	0.66	0.62	0.48	0.74	0.65	0.56	1.15	0.38
Yheavies	0.17	0.21	0.09	0.12	0.13	0.10	0.09	0.14	0.12	0.11	0.21	0.07
Sether	1.08	1.14	1.39	1.34	1.41	1.21	0.96	1.24	1.40	1.34	1.42	1.22
Yether	0.24	0.26	0.27	0.27	0.27	0.19	0.19	0.24	0.26	0.26	0.26	0.23

Table 0.23: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-33	WC-34	WC-35	WC-36	WC-37	WC-38	WC-39	WC-40	WC-41	WC-42	WC-43
Time on Stream	172:01:34	174:01:34	176:01:34	178:01:34	179:57:34	183:55:37	193:01:37	194:01:37	195:01:37	196:01:37	196:59:37
Entry Temperature	92	93	94	94	94	93	90	91	91	89	88
Temperature	274	274	274	274	275	276	275	275	275	275	275
WHSV	0.3	0.3	0.3	0.3	0.3	0.3	1.28	1.28	1.28	1.28	1.28
Pump Rate (ml/min)	0.037	0.037	0.037	0.037	0.037	0.037	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3
Conversion	39.43	42.60	45.03	38.70	37.40	36.22	19.33	18.08	17.73	18.02	15.67
Thymol Selectivity	65.05	65.42	64.61	64.06	65.86	63.97	57.76	57.31	57.78	57.18	57.07
Thymol Yield	25.65	27.87	29.09	24.79	24.63	23.17	11.17	10.36	10.24	10.31	8.94
S3-isopropyl-5-methylphenol	**4.91**	**4.69**	**4.84**	**4.76**	**4.57**	**5.19**	**2.24**	**2.09**	**2.08**	**2.07**	**1.81**
Y3-methyl-5-isopropylphenol	1.93	2.00	2.18	1.84	1.71	1.88	0.43	0.38	0.37	0.37	0.28
S4-isopropyl-3-methylphenol	**9.53**	**9.32**	**9.34**	**9.76**	**9.61**	**9.37**	**11.06**	**10.65**	**10.66**	**10.98**	**10.19**
Y3-methyl-4-isopropylphenol	3.76	3.97	4.21	3.78	3.59	3.39	2.14	1.92	1.89	1.98	1.60
S2-isopropyl-3-methylphenol	**5.05**	**4.91**	**4.42**	**4.81**	**5.03**	**5.54**	**15.84**	**16.65**	**16.66**	**16.90**	**18.10**
Y3-methyl-2-isopropylphenol	1.99	2.09	1.99	1.86	1.88	2.00	3.06	3.01	2.95	3.05	2.84
Thymol	76.95	77.56	77.65	76.82	77.42	76.09	66.47	66.11	66.28	65.62	65.48
3-methyl-5-isopropylphenol	5.80	5.56	5.82	5.71	5.37	6.18	2.57	2.41	2.38	2.38	2.07
3-methyl-2-isopropylphenol	11.28	11.06	11.22	11.71	11.29	11.15	12.72	12.28	12.22	12.60	11.68
3-methyl-4-isopropylphenol	5.97	5.83	5.31	5.77	5.92	6.58	18.23	19.20	19.11	19.40	20.76
STotal.Isomer	**84.54**	**84.35**	**83.21**	**83.39**	**85.07**	**84.07**	**86.90**	**86.69**	**87.17**	**87.14**	**87.16**
YTotal.Isomer	33.33	35.93	37.47	32.27	31.82	30.45	16.80	15.67	15.46	15.71	13.66
Slights	1.20	1.38	1.22	1.18	1.22	1.23	1.34	1.32	1.30	1.26	1.30
Ylights	0.47	0.59	0.55	0.46	0.46	0.45	0.26	0.24	0.23	0.23	0.20
SC-10	0.55	0.54	0.54	0.53	0.53	0.54	0.29	0.27	0.05	0.19	0.31
YC-10	0.22	0.23	0.24	0.20	0.20	0.20	0.06	0.05	0.01	0.04	0.05
Sdi-isopropylated	9.36	9.37	10.50	10.37	8.84	9.35	4.45	4.30	3.97	4.05	3.34
Ydi-isopropylated	3.69	3.99	4.73	4.01	3.31	3.39	0.86	0.78	0.70	0.73	0.52
Sheavies	0.62	0.67	0.72	0.65	0.59	0.79	0.48	0.52	0.45	0.64	0.19
Yheavies	0.25	0.29	0.33	0.25	0.22	0.29	0.09	0.09	0.08	0.12	0.03
Sether	0.40	0.38	0.39	0.41	0.41	0.43	1.26	1.59	1.35	1.37	1.85
Yether	0.16	0.16	0.17	0.16	0.15	0.16	0.24	0.29	0.24	0.25	0.29

Table 0.24: Conversion, selectivity and yield data for simulated washcoating (cont.)

	WC-44	WC-45	WC-46	WC-47	WC-48	WC-49	WC-50	WC-51	WC-52	WC-53	WC-54	WC-55
Time on Stream	201:01:37	202:01:37	203:01:37	204:01:37	206:01:37	207:01:37	207:31:37	208:01:37	208:31:12	217:01:12	218:01:12	219:01:12
Entry Temperature	88	89	89	88	84	83	83	83	83	90	91	91
Temperature	275	275	275	275	274	274	275	275	275	275	275	274
WHSV	1.81	181	1.81	1.81	3.63	3.63	3.63	3.63	3.63	1.28	1.28	1.28
Pump Rate (ml/min)	0.227	0.227	0.227	0.227	0.454	0.454	0.454	0.454	0.454	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	12.90	12.14	11.78	11.65	7.75	7.52	7.79	7.13	7.59	11.50	11.56	12.10
Thymol Selectivity	51.43	50.96	49.51	49.67	36.55	33.74	34.50	33.18	35.30	39.60	39.39	39.85
Thymol Yield	6.63	6.19	5.83	5.78	2.83	2.54	2.69	2.37	2.68	4.55	4.55	4.82
S3-isopropyl-5-methylphenol	**1.65**	**1.55**	**1.51**	**1.38**	**1.08**	**0.77**	**0.76**	**0.67**	**0.79**	**0.78**	**0.89**	**0.89**
Y3-methyl-5-isopropylphenol	0.21	0.19	0.18	0.16	0.08	0.06	0.06	0.05	0.06	0.09	0.10	0.11
S4-isopropyl-3-methylphenol	**10.52**	**10.34**	**9.47**	**9.71**	**8.09**	**6.28**	**6.07**	**5.37**	**5.85**	**6.19**	**6.51**	**6.47**
Y3-methyl-4-isopropylphenol	1.36	1.25	1.11	1.13	0.63	0.47	0.47	0.38	0.44	0.71	0.75	0.78
S2-isopropyl-3-methylphenol	**22.06**	**22.42**	**22.81**	**23.57**	**22.03**	**21.57**	**22.47**	**22.06**	**23.53**	**23.76**	**23.50**	**23.47**
Y3-methyl-2-isopropylphenol	2.84	2.72	2.69	2.74	1.71	1.62	1.75	1.57	1.78	2.73	2.72	2.84
Thymol	60.05	59.77	59.44	58.90	53.95	54.11	54.08	54.14	53.92	56.31	56.03	56.38
3-methyl-5-isopropylphenol	1.93	1.82	1.81	1.64	1.59	1.24	1.19	1.09	1.21	1.11	1.27	1.27
3-methyl-2-isopropylphenol	12.28	12.12	11.36	11.52	11.94	10.07	9.52	8.77	8.93	8.80	9.26	9.15
3-methyl-4-isopropylphenol	25.75	26.29	27.39	27.95	32.52	34.59	35.21	36.00	35.94	33.78	33.43	33.20
STotal.Isomer	**85.65**	**85.27**	**83.30**	**84.33**	**67.75**	**62.35**	**63.80**	**61.28**	**65.46**	**70.33**	**70.30**	**70.69**
YTotal.Isomer	11.05	10.35	9.81	9.82	5.25	4.69	4.97	4.37	4.97	8.09	8.13	8.55
Slights	1.34	1.49	1.34	1.73	1.79	2.04	1.79	1.74	2.09	1.58	1.53	1.67
Ylights	0.17	0.18	0.16	0.20	0.14	0.15	0.14	0.12	0.16	0.18	0.18	0.20
SC-10	0.18	0.17	0.15	0.16	-	-	-	-	-	-	-	-
YC-10	0.02	0.02	0.02	0.02	-	-	-	-	-	-	-	-
Sdi-isopropylated	2.94	2.71	2.69	2.32	1.57	1.25	1.29	1.21	1.07	1.84	1.87	2.06
Ydi-isopropylated	0.38	0.33	0.32	0.27	0.12	0.09	0.10	0.09	0.08	0.21	0.22	0.25
Sheavies	0.73	0.60	1.17	0.44	0.99	1.42	1.54	1.72	1.69	0.94	1.43	1.17
Yheavies	0.09	0.07	0.14	0.05	0.08	0.11	0.12	0.12	0.13	0.11	0.17	0.14
Sether	2.83	3.21	4.55	4.37	19.04	23.81	22.63	24.41	20.53	18.32	18.42	18.26
Yether	0.37	0.39	0.54	0.51	1.47	1.79	1.76	1.74	1.56	2.11	2.13	2.21

Table 0.25: GC raw data for H-MFI-90 powder

		PW-1	PW-2	PW-3	PW-4	PW-6	PW-9	PW-12	PW-17	PW-19	PW-23	PW-25	PW-29	PW-32
Time on Stream		1:02:06	2:01:00	3:01:00	4:01:00	7:01:00	15:01:00	25:01:00	35:01:00	46:01:00	59:37:00	71:01:00	79:01:00	89:45:00
Entry Temperature		103	103	96	88	90	90	88	86	92	87	86	86	86
Temperature		274	276	276	276	277	275	275	275	275	275	275	275	274
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	3.7		4.2	8.6	7.6	6.6	21.2	37.1	54.9	47.2	49.7	63.2	58.9
???	± 5.04	6.8	3.2	3.9	4.3		3.5							
phenol	± 5.26	31.5			0.6	3.2		4	16.9	11.7	10.2	9.7	11.2	11.6
o-Cresol	± 5.35	170.9	17.6	12.8	8	13	12.3	4.1		10.3	7.9	7.9	10.2	8.7
p-Cresol	± 5.60	397.2	69.6	48.5	28.4	70.3	60.7	47.5	87.6	106.2	84.9	85.6	107.1	97.8
m-Cresol	± 5.80	9066.9	3430.2	3213.7	4541.7	6226.4	4924.9	5713.6	11250	13793.5	11671.2	11789.5	15149.3	13795.5
???	± 6.00	19.6	3.4	3.1	4.2	5.6	4	4.2	7.4	10.3	8.7	8	10.7	8.4
2,4-Xylenol	± 6.20	36	5.8	4.6	4.8	5.4	4.5	2.9	2.6	3.1	2	2.5	2.4	2.8
2,5-Xylenol	± 6.50	7.5	3.6	1.8	4.7	6.3	4.4	3.4	6.5	10.5	5.8	5.2	6.7	6.7
2,3-Xylenol	± 6.74	31.7	5.3	1.6	6.3	8	5.4	4.2	5.7	8.5	5	5	4.2	4.4
???	± 6.90	53.4	12.8	5.4	13.6	13	11.7	3.6	5.5	5.8	3.6	2.7	2.5	3.4
???	± 7.03			10.4										
???	± 7.16	73.6	16.2	10.5	11.1	9.3	12.1	2.1	2.4	2.6	1.7	1.5	1.8	2.1
2-Isopropyl-4-methyl Phenol	± 7.30	57.1		13.8	23.1	28.4	21.9	14.2	19.4	21.7	13.4	12.1	13.6	12.6
???	± 7.49	13.6	2.9	2.7	2.8	5.2	4.3	1.1	1.6	3.4	0.7	1.9	2	1.5
Thymol isomer (2,3)	± 7.60	32.2	34.5	68.5	142.6	231.6	120.2	240.8	379	477.5	314	295.8	358	336.8
???	± 7.73	142.8	41.5	32	42	43.5	41	14.1	17.1	20	12.2	10.5	12.2	11.3
Thymol	± 7.90	1232.1	989.1	1522.3	3048.4	4428.4	2868.8	2429.6	3329.9	3978	2347.1	2093.6	2488.5	2318.9
????	± 8.19	163.7	44.2	35.8	48.6	52.8	42.6	18.8	23.3	26.9	15.5	13.3	16.7	14.9
????	± 8.33	689.6	304.1	299.1	449.6	526	405.7	172.3	219.4	243.5	145.8	124.3	145.9	135.5
6-n-Propyl-3-Methyl Phenol	± 8.40	5.7	7.5	17	40.3	65.2	34	41.2	47.2	60.6	31.8	26.8	30.6	29.5
2,6-Diisoprop.-3-Met. Phen.	± 8.55	276.9	76.8	62.5	80.3	82.4	65	23	27.7	30.6	17.6	15.1	17.8	16.9
5,3 Thymol isomer	± 8.67	308.6	121.6	133.3	238.4	313.1	260.6	128.6	166.6	191.1	106.8	92.9	110.6	102.4
4,3 Thymol isomer	± 8.78	276.6	227.5	347.8	728.1	1152.4	693.8	737.9	1013.2	1224.4	681.5	612.2	716.4	676.6
C-13 fraction (13.02)	± 8.83	32.1	5.6	5.2	4	2.6	4.2						4.4	
????	± 9.22	156.1	66.1	60.6	89.8	78.3	85.9	10	8.1	10.9	4.4	2.9	14.5	4.1
????	± 9.48	120.7	36.1	28.1	41.9	43.6	41.9	15.8	19.9	25.1	12.7	10.1	2.6	12.4
????	± 9.60	17.3	4.1	3.8	4.1	2.4	4.7			2.3	2.1	1.9		
????	± 10.30	326.6	124.4	94	122.4	91.7	112	6.4	4.2	5.7	3.2	2.4		
????	± 10.70	78.7	19.8	11.4	10.5	7	13.4							
4,6-Diisoprop.-3-Met. Phen.	± 11.18	80.4	59	87.6	199.2	256.8	190	93.6	97.5	119.9	56.6	47.2	53.5	50.1
????	± 11.30	13												
????	± 11.56	46.9	20.1	12.7	14.6	6.5	2.7							
????	± 11.87													
????	± 12.21	11.3	5.5	7.2	13	13.6	10	5.9	5.9	8.8	3.7	2.5	3.5	4.2
5,6-Diisoprop.-3-Met. Phen.	± 12.70	56.8	24.8	27	39.2	48.5	32.8	21.6	24.1	32.6	15.1	14.6	13.9	13.8
Heavies	± 13.04	85.8	44.5	37.8	61.6	42.8	57.3	4.4						
Heavies		86.7	52.3	52.1	2078.3	73.9	105.8	36.5	18	23.1	13.2	27	11.5	8.2

Table 0.26: GC raw data for H-MFI-90 powder

		PW-35	PW-36	PW-37	PW-38	PW2-40	PW-41	PW-42	PW-43	PW-44	PW-45	PW-46
Time on Stream		92:01:00	93:01:00	94:01:00	95:01:00	97:01:00	98:01:00	103:01:00	103:31:00	104:01:00	104:31:00	105:01:00
Entry Temperature		88	88	88	88	88	88	83	83	84	84	84
Temperature		275	275	275	275	275	274	275	274	274	275	275
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	1.81	1.81	1.81	1.81	1.81
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.302	0.302	0.302	0.302	0.302
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	36.3	51.7	47.4	58.9	59.2	49.8	51.5	59.2	60	74.7	64.2
???	± 5.04										0.8	
phenol	± 5.26	6.7	9.4	8.4	10.7	11.5	9.5	5.8	6.2	9.4	8.7	6.7
o-Cresol	± 5.35	4.3	7.5	6.6	8.8	8.8	6.9	6.3	7.8	7.4	9.8	7.9
p-Cresol	± 5.60	52.4	79.7	70.1	93.2	92.8	75	67	80.5	80.1	102.6	85.6
m-Cresol	± 5.80	7466.4	11371.5	10052.6	13365.2	13225.7	10727.8	10088	12224.9	12145.9	15637.7	13003.1
???	± 6.00	4.9	7.7	7.1	9.2	9.4	7.9	6	7.4	6.7	8.8	7.6
2,4-Xylenol	± 6.20	0.9	2.2	1.4	1.4	2.4	1.2	1.3	1.6	1.4	1.9	1.4
2,5-Xylenol	± 6.50	2.8	5.3	4.7	5.5	5.7	4.6	4.2	4.4	4.2	6.1	4.9
2,3-Xylenol	± 6.74	2.2	3	2.6	3.1	3.9	2.3	1.2	1.1	0.8	1.4	1.3
???	± 6.90		0.9	1.9	2	2.6	2					
???	± 7.03											
???	± 7.16		1	0.8	1.7	1.2	1.3		0.2			
2-Isopropyl-4-methyl Phenol	± 7.30	6.8	8.8	7.5	9.4	10.4	7.7	3.2	3.6	3.6	4.8	3.8
???	± 7.49		0.9			1.4						
Thymol isomer (2,3)	± 7.60	173	250.8	215.1	279.3	278.7	224	106.8	120.4	121.5	147.9	122.4
???	± 7.73	5.5	7.7	7	8.6	8.9	4.9	2.8	3.3	3.2	3.5	2.9
Thymol	± 7.90	1109	1623.7	1367.7	1793.3	1783.7	1426.4	567.4	630.7	633.4	780	642.2
????	± 8.19	6.5	10.3	8.2	11.1	11.1	8.9	3.3	3.4	3.6	4.8	3.7
????	± 8.33	62.9	91.4	77.2	101	101	81.3	29.4	32.9	32.3	40.1	33.2
6-n-Propyl-3-Methyl Phenol	± 8.40	14.5	19.8	17.7	21.4	21.1	17	4.2	5.3	4.7	5.7	4.6
2,6-Diisoprop.-3-Met. Phen.	± 8.55	7.6	11.4	9.7	12.5	12.3	9.9	3.9	4.7	4.2	5.5	4.7
5,3 Thymol isomer	± 8.67	49.2	71.3	60.1	79.5	79.6	63.3	25.1	28.4	28.3	34.8	28.5
4,3 Thymol isomer	± 8.78	322.7	473.4	391	521	517	406.4	172.6	192.8	197.4	240.9	198.2
C-13 fraction (13.02)	± 8.83											
????	± 9.22	1.7	3	2.8	2.3	2.3	1.7					
????	± 9.48	5.1	9.4	8.5	9.2	9.6	7.8	2.6	3.1	3.4	4.7	3.8
????	± 9.60											
????	± 10.30											
????	± 10.70											
4,6-Diisoprop.-3-Met. Phen.	± 11.18	25	33.2	28.5	35.8	35.3	27.9	6.4	7.8	8.6	8.4	6.9
????	± 11.30											
????	± 11.80											
????	± 12.09											
????	± 12.21	1.1	2.2	1.8	2.1	1.9	2					
5,6-Diisoprop.-3-Met. Phen.	± 12.70	5.3	8.4	6.8	9.8	10	7.3	1.1	2	2.4	2.5	2.2
Heavies	± 13.04											
Heavies		9.5	9.8	14.3	12.6	19.2	6.2	24.1	24.4	14.4	19.3	8.3

Table 0.27: GC raw data for H-MFI-90 powder (cont.)

		PW-47	PW-48	PW-49	PW-50	PW-51	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59
Time on Stream		116:31:00	117:01:00	117:31:00	118:01:00	127:01:00	135:01:00	137:01:00	139:01:00	141:01:00	141:31:00	180:53:22	188:56:55	190:00:55
Entry Temperature		87	85	85	85	88	86	86	86	86	86	86	89	90
Temperature		274	274	275	275	275	275	274	275	275	275	275	276	276
WHSV		3.62	3.62	3.62	3.62	3.62	0.3	0.3	0.3	0.3	0.3	0.96	0.96	0.96
Pump Rate (ml/min)		0.604	0.604	0.604	0.604	0.604	0.05	0.05	0.05	0.05	0.05	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	97.8	47.9	40.2	42.3	30.5	33.7	24.8	40.3	17.7	24.2	31.4	34.7	60.5
???	± 5.04	1.1	0.9	0.7	0.4	0.8	1	0.9	1.8	1.2	1	0.6	1	0.9
phenol	± 5.26	2.5	3.2	1.6	1.1	1.2	6.4	4.4	7.3	3.7	5	4.5	5.1	9.6
o-Cresol	± 5.35	11	4.9	4.4	5.7	3.7	8.5	5.9	11.8	3.7	5.7	5.3	5.8	12.9
p-Cresol	± 5.60	112.5	59.1	50.9	58.9	44.1	84.9	64.1	115.5	45.2	66.5	57.7	64.2	132.2
m-Cresol	± 5.80	17754.9	9307.6	7978.2	9210.1	6899.4	10765.8	8195.7	14987.4	5715	8453.8	8447.7	9419.8	19487.7
???	± 6.00	10.3	5.3	5	5.6	4.1	7.5	5.9	10.6	4.4	6.4	5.5	6.4	5.4
2,4-Xylenol	± 6.20	1.7	1.3	1.4	1.1	1.1	4.2	4.4	6.7	3.3	5.4	2.4	1.4	2.3
2,5-Xylenol	± 6.50	5.3	3.1	3.2	3.5	2.3	6.3	5.9	9.5	3.2	5.7	3.7	4.1	9.5
2,3-Xylenol	± 6.74						4.1	4.4	5.5	2.8	3.9	1.8	1.4	2.5
???	± 6.90						5.9	4.4	7.9	2.8	4.3	1.4	1.1	2.6
???	± 7.03										0.8			
???	± 7.16						3.9	3	6	2.8	3.2	2.5	0.7	1.4
2-Isopropyl-4-methyl Phenol	± 7.30	2.8					21.7	16.1	26.6	11.9	17.6	5.5	5.3	9.1
???	± 7.49						1.8	1.7	3.2	1.4	1.8	1	1.2	1.4
Thymol isomer (2,3)	± 7.60	29.3	13.6	10.4	11.3	11.7	384	289.4	459.2	207.3	308.3	154.9	165.4	276.8
???	± 7.73						20.8	15.2	26	11.2	15.9	5.7	5.2	9
Thymol	± 7.90	123.6	53.8	42	41.4	44.1	3613.1	2659	4464.3	1920.4	2847.7	958	958.8	1650.1
????	± 8.19	1.2					23.5	17.5	29	12.8	17.7	5.7	5.4	3.8
????	± 8.33	4.5	2.4	1.4	1.2	2.6	231.5	173.8	296.7	127.8	183.1	59.1	57.4	102.1
6-n-Propyl-3-Methyl Phenol	± 8.40						68.4	51.5	80.8	40	53.7	13.5	11	14.4
2,6-Diisoprop.-3-Met. Phen.	± 8.55						26	19.8	33.4	14.8	20.4	7	6.6	11.5
5,3 Thymol isomer	± 8.67	6.5	2.6	2.2	2.1	2.3	162.8	124.4	213.1	93	127.7	44.4	41.5	67.2
4,3 Thymol isomer	± 8.78	44.7	19.1	14.4	14.4	13.7	762.9	588.4	976.5	428.1	634.7	262.3	255.2	423.8
C-13 fraction (13.02)	± 8.83							0.7	0.5	0.3	0.4			
????	± 9.22						11.4	7.4	14.8	6.6	8.2	1.9	0.7	1.3
????	± 9.48						20.9	16.4	27.2	11.3	17.8	6.4	5	8.2
????	± 9.60						2.1	1.4	1.6		1.7			
????	± 10.30						7.9	5.6	8.2	5.5	6.8			
????	± 10.70													
4,6-Diisoprop.-3-Met. Phen.	± 11.18	1.2	1	1.1	1.2	1.2	133.5	105.7	191.8	84.3	108.7	28.7	19.8	24.7
????	± 11.30													
????	± 11.80													
????	± 12.09													
????	± 12.21						6.9	5	6.2	6.2	6.4	1.1		
5,6-Diisoprop.-3-Met. Phen.	± 12.70						21.2	16.7	29	14.9	23.7	4.3	4.4	8.6
Heavies	± 13.04						3.3	4	5.3	2.8				
Heavies		10.9	12.5	11.9	15.5	21.4	12	20.9	14.4	19.4	21.6	9	13.3	14.6

Table 0.28: Product composition (%) for H-MFI-90 powder

		PW-1	PW-2	PW-3	PW-4	PW-6	PW-9	PW-12	PW-17	PW-19	PW-23	PW-25	PW-29	PW-32
Time on Stream		1:02:06	2:01:00	3:01:00	4:01:00	7:01:00	15:01:00	25:01:00	35:01:00	46:01:00	59:37:00	71:01:00	79:01:00	89:45:00
Entry Temperature		103	103	96	88	90	90	88	86	92	87	86	86	86
Temperature		274	276	276	276	277	275	275	275	275	275	275	275	274
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	3	2	2	2	2	2	2	2
ether	± 4.70	0.02	-	0.06	0.07	0.05	0.06	0.18	0.18	0.21	0.24	0.25	0.25	0.26
???	± 5.04	0.05	0.06	0.07	0.05	-	0.04	-	-	-	-	-	-	-
phenol	± 5.26	0.18	-	-	0.00	0.02	-	0.03	0.08	0.05	0.05	0.05	0.04	0.05
o-Cresol	± 5.35	1.36	0.35	0.24	0.09	0.11	0.14	0.05	-	0.06	0.05	0.06	0.06	0.05
p-Cresol	± 5.60	3.16	1.38	0.92	0.30	0.61	0.71	0.56	0.58	0.58	0.59	0.60	0.59	0.59
m-Cresol	± 5.80	72.12	67.87	61.06	48.66	54.41	57.93	67.07	74.57	74.92	80.99	82.66	83.80	83.46
???	± 6.00	0.12	0.05	0.05	0.03	0.04	0.04	0.04	0.04	0.04	0.05	0.04	0.05	0.04
2,4-Xylenol	± 6.20	0.22	0.09	0.07	0.04	0.04	0.04	0.03	0.01	0.01	0.01	0.01	0.01	0.01
2,5-Xylenol	± 6.50	0.05	0.05	0.03	0.04	0.04	0.04	0.03	0.03	0.04	0.03	0.03	0.03	0.03
2,3-Xylenol	± 6.74	0.19	0.08	0.02	0.05	0.05	0.05	0.04	0.03	0.04	0.03	0.03	0.02	0.02
???	± 6.90	0.33	0.19	0.08	0.11	0.09	0.11	0.03	0.03	0.02	0.02	0.01	0.01	0.02
???	± 7.03	-	-	0.15	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.45	0.25	0.15	0.09	0.06	0.11	0.02	0.01	0.01	0.01	0.01	0.01	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.35	-	0.20	0.19	0.19	0.20	0.13	0.10	0.09	0.07	0.06	0.06	0.06
???	± 7.49	0.08	0.04	0.04	0.02	0.03	0.04	0.01	0.01	0.01	0.00	0.01	0.01	0.01
Thymol isomer (2,3)	± 7.60	0.18	0.47	0.89	1.05	1.39	0.97	1.94	1.72	1.78	1.49	1.42	1.36	1.40
???	± 7.73	0.78	0.56	0.42	0.31	0.26	0.33	0.11	0.08	0.07	0.06	0.05	0.05	0.05
Thymol	± 7.90	6.72	13.42	19.84	22.40	26.54	23.15	19.56	15.14	14.82	11.17	10.07	9.44	9.62
????	± 8.19	0.89	0.60	0.47	0.36	0.32	0.34	0.15	0.11	0.10	0.07	0.06	0.06	0.06
????	± 8.33	3.76	4.13	3.90	3.30	3.15	3.27	1.39	1.00	0.91	0.69	0.60	0.55	0.56
6-n-Propyl-3-Methyl Phenol	± 8.40	0.03	0.10	0.22	0.30	0.39	0.27	0.33	0.21	0.23	0.15	0.13	0.12	0.12
2,6-Diisoprop.-3-Met. Phen.	± 8.55	1.15	0.79	0.62	0.45	0.38	0.40	0.14	0.10	0.09	0.06	0.06	0.05	0.05
5,3 Thymol isomer	± 8.67	1.68	1.65	1.74	1.75	1.88	2.10	1.04	0.76	0.71	0.51	0.45	0.42	0.42
4,3 Thymol isomer	± 8.78	1.51	3.09	4.53	5.35	6.91	5.60	5.94	4.61	4.56	3.24	2.94	2.72	2.81
C-13 fraction (13.02)	± 8.83	0.13	0.06	0.05	0.02	0.01	0.03	-	-	-	-	-	0.01	-
????	± 9.22	0.65	0.68	0.60	0.50	0.36	0.53	0.06	0.03	0.03	0.02	0.01	0.04	0.01
????	± 9.48	0.50	0.37	0.28	0.23	0.20	0.26	0.10	0.07	0.07	0.05	0.04	0.01	0.04
????	± 9.60	0.07	0.04	0.04	0.02	0.01	0.03	-	-	0.01	0.01	0.01	-	-
????	± 10.30	1.36	1.28	0.93	0.68	0.42	0.69	0.04	0.01	0.02	0.01	0.01	-	-
????	± 10.70	0.33	0.20	0.11	0.06	0.03	0.08	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.33	0.61	0.87	1.11	1.17	1.17	0.57	0.34	0.34	0.20	0.17	0.15	0.16
????	± 11.30	0.05	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	0.19	0.21	0.13	0.08	0.03	0.02	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.05	0.06	0.07	0.07	0.06	0.06	0.04	0.02	0.02	0.01	0.01	0.01	0.01
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.24	0.26	0.27	0.22	0.22	0.20	0.13	0.08	0.09	0.05	0.05	0.04	0.04
Heavies	± 13.04	0.36	0.46	0.37	0.34	0.20	0.35	0.03	-	-	-	-	-	-
Heavies		0.36	0.54	0.52	11.62	0.34	0.65	0.22	0.06	0.07	0.05	0.10	0.03	0.03

Table 0.29: Product composition (%) for H-MFI-90 powder

		PW-35	PW-36	PW-37	PW-38	PW2-40	PW-41	PW-42	PW-43	PW-44	PW-45	PW-46
Time on Stream		92:01:00	93:01:00	94:01:00	95:01:00	97:01:00	98:01:00	103:01:00	103:31:00	104:01:00	104:31:00	105:01:00
Entry Temperature		88	88	88	88	88	88	83	83	84	84	84
Temperature		275	275	275	275	275	274	275	274	274	275	275
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	1.81	1.81	1.81	1.81	1.81
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.302	0.302	0.302	0.302	0.302
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.30	0.28	0.29	0.27	0.28	0.29	0.34	0.33	0.33	0.32	0.33
???	± 5.04	-	-	-	-	-	-	-	-	-	0.00	-
phenol	± 5.26	0.05	0.05	0.05	0.05	0.05	0.05	0.04	0.03	0.05	0.04	0.03
o-Cresol	± 5.35	0.05	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06
p-Cresol	± 5.60	0.60	0.60	0.60	0.60	0.60	0.60	0.62	0.61	0.62	0.61	0.62
m-Cresol	± 5.80	84.92	85.41	85.94	86.13	86.02	86.26	92.89	93.36	93.32	93.57	93.64
???	± 6.00	0.04	0.04	0.05	0.05	0.05	0.05	0.04	0.04	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
2,5-Xylenol	± 6.50	0.02	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.02	0.03	0.03
2,3-Xylenol	± 6.74	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.00	0.01	0.01
???	± 6.90	-	0.01	0.01	0.01	0.01	0.01	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	-	0.01	0.01	0.01	0.01	0.01	-	0.00	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	0.06	0.05	0.05	0.05	0.05	0.05	0.02	0.02	0.02	0.02	0.02
???	± 7.49	-	0.01	-	-	0.01	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	1.35	1.29	1.26	1.23	1.24	1.24	0.67	0.63	0.64	0.61	0.60
???	± 7.73	0.04	0.04	0.04	0.04	0.04	0.03	0.02	0.02	0.02	0.01	0.01
Thymol	± 7.90	8.65	8.36	8.02	7.93	7.96	7.87	3.58	3.30	3.34	3.20	3.17
????	± 8.19	0.05	0.05	0.05	0.05	0.05	0.05	0.02	0.02	0.02	0.02	0.02
????	± 8.33	0.49	0.47	0.45	0.45	0.45	0.45	0.19	0.17	0.17	0.16	0.16
6-n-Propyl-3-Methyl Phenol	± 8.40	0.11	0.10	0.10	0.09	0.09	0.09	0.03	0.03	0.02	0.02	0.02
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.05	0.04	0.04	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02
5,3 Thymol isomer	± 8.67	0.38	0.37	0.35	0.35	0.36	0.35	0.16	0.15	0.15	0.14	0.14
4,3 Thymol isomer	± 8.78	2.52	2.44	2.29	2.30	2.31	2.24	1.09	1.01	1.04	0.99	0.98
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-	-
????	± 9.22	0.01	0.01	0.01	0.01	0.01	0.01	-	-	-	-	-
????	± 9.48	0.03	0.04	0.04	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.01
????	± 9.60	-	-	-	-	-	-	-	-	-	-	-
????	± 10.30	-	-	-	-	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.15	0.13	0.13	0.12	0.12	0.12	0.03	0.03	0.03	0.03	0.03
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.01	0.01	0.01	0.01	0.01	0.01	-	-	-	-	-
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.03	0.03	0.03	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.01
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-	-
Heavies		0.06	0.04	0.06	0.04	0.07	0.03	0.12	0.10	0.06	0.06	0.03

Table 0.30: Product composition (%) for H-MFI-90 powder (cont.)

		PW-47	PW-48	PW-49	PW-50	PW-51	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59
Time on Stream		116:31:00	117:01:00	117:31:00	118:01:00	127:01:00	135:01:00	137:01:00	139:01:00	141:01:00	141:31:00	180:53:22	188:56:55	190:00:55
Entry Temperature		87	85	85	85	88	86	86	86	86	86	86	89	90
Temperature		274	274	275	275	275	275	274	275	275	275	275	276	276
WHSV		3.62	3.62	3.62	3.62	3.62	0.3	0.3	0.3	0.3	0.3	0.96	0.96	0.96
Pump Rate (ml/min)		0.604	0.604	0.604	0.604	0.604	0.05	0.05	0.05	0.05	0.05	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.39	0.36	0.36	0.32	0.31	0.17	0.16	0.15	0.16	0.15	0.24	0.24	0.20
???	± 5.04	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00
phenol	± 5.26	0.01	0.02	0.01	-	0.01	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
o-Cresol	± 5.35	0.06	0.05	0.05	0.06	0.05	0.06	0.05	0.06	0.05	0.05	0.06	0.05	0.06
p-Cresol	± 5.60	0.62	0.62	0.63	0.63	0.63	0.58	0.58	0.58	0.58	0.57	0.60	0.61	0.62
m-Cresol	± 5.80	98.00	98.12	98.17	98.29	98.02	73.38	73.72	75.42	72.90	73.06	87.85	88.96	90.69
???	± 6.00	0.04	0.04	0.05	0.05	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.01	0.02	0.03	0.03	0.03	0.04	0.02	0.01	0.01
2,5-Xylenol	± 6.50	0.02	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.03	0.04	0.03	0.03	0.03
2,3-Xylenol	± 6.74	-	-	-	-	-	0.02	0.03	0.02	0.03	0.03	0.01	0.01	0.01
???	± 6.90	-	-	-	-	-	0.03	0.03	0.03	0.03	0.03	0.01	0.01	0.01
???	± 7.03	-	-	-	-	-	-	-	-	-	0.01	-	-	-
???	± 7.16	-	-	-	-	-	0.02	0.02	0.02	0.03	0.02	0.02	0.01	0.00
2-Isopropyl-4-methyl Phenol	± 7.30	0.01	-	-	-	-	0.11	0.11	0.10	0.12	0.12	0.04	0.04	0.03
???	± 7.49	-	-	-	-	-	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Thymol isomer (2,3)	± 7.60	0.11	0.10	0.09	0.08	0.11	1.80	1.79	1.58	1.81	1.83	1.10	1.07	0.88
???	± 7.73	-	-	-	-	-	0.10	0.09	0.09	0.10	0.09	0.04	0.03	0.03
Thymol	± 7.90	0.47	0.39	0.35	0.30	0.43	16.89	16.40	15.41	16.80	16.88	6.83	6.21	5.27
????	± 8.19	0.00	-	-	-	-	0.11	0.11	0.10	0.11	0.10	0.04	0.03	0.01
????	± 8.33	0.02	0.02	0.01	0.01	0.03	1.08	1.07	1.02	1.12	1.09	0.42	0.37	0.33
6-n-Propyl-3-Methyl Phenol	± 8.40	-	-	-	-	-	0.32	0.32	0.28	0.35	0.32	0.10	0.07	0.05
2,6-Diisoprop.-3-Met. Phen.	± 8.55	-	-	-	-	-	0.09	0.09	0.09	0.10	0.09	0.04	0.03	0.03
5,3 Thymol isomer	± 8.67	0.02	0.02	0.02	0.02	0.02	0.76	0.77	0.74	0.81	0.76	0.32	0.27	0.21
4,3 Thymol isomer	± 8.78	0.17	0.14	0.12	0.11	0.13	3.57	3.63	3.37	3.75	3.76	1.87	1.65	1.35
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	0.00	0.00	0.00	0.00	-	-	-
????	± 9.22	-	-	-	-	-	0.04	0.03	0.04	0.04	0.04	0.01	0.00	0.00
????	± 9.48	-	-	-	-	-	0.07	0.08	0.07	0.08	0.08	0.03	0.02	0.02
????	± 9.60	-	-	-	-	-	0.01	0.01	0.00	0.00	0.01	-	-	-
????	± 10.30	-	-	-	-	-	0.03	0.03	0.02	0.04	0.03	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.00	0.01	0.01	0.01	0.01	0.47	0.50	0.50	0.56	0.49	0.16	0.10	0.06
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	-	-	-	-	-	0.02	0.02	0.02	0.04	0.03	0.01	-	-
5,6-Diisoprop.-3-Met. Phen.	± 12.70	-	-	-	-	-	0.08	0.08	0.08	0.10	0.11	0.02	0.02	0.02
Heavies	± 13.04	-	-	-	-	-	0.01	0.02	0.01	0.02	-	-	-	-
Heavies		0.03	0.07	0.08	0.09	0.16	0.04	0.10	0.04	0.13	0.10	0.05	0.07	0.04

Table 0.31: Conversion, selectivity and yield data for H-MFI-90 powder

	PW-1	PW-2	PW-3	PW-4	PW-6	PW-9	PW-12	PW-17	PW-19	PW-23	PW-25	PW-29	PW-32
Time on Stream	1:02:06	2:01:00	3:01:00	4:01:00	7:01:00	15:01:00	25:01:00	35:01:00	46:01:00	59:37:00	71:01:00	79:01:00	89:45:00
Entry Temperature	103	103	96	88	90	90	88	86	92	87	86	86	86
Temperature	274	276	276	276	277	275	275	275	275	275	275	275	274
$WHSV_{Wet}$	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (mL/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guage Pressure (bar)	2	2	2	2	2	3	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3		3	3	3	3	3	3	3
Conversion	27.88	32.13	38.94	51.34	45.59	42.07	32.93	25.43	25.08	19.01	17.34	16.20	16.54
Thymol Selectivity	24.11	41.77	50.94	43.64	58.21	55.02	59.40	59.53	59.09	58.77	58.06	58.28	58.18
Thymol Yield	6.72	13.42	19.84	22.40	26.54	23.15	19.56	15.14	14.82	11.17	10.07	9.44	9.62
S3-isopropyl-5-methylphenol	**6.04**	**5.14**	**4.46**	**3.41**	**4.12**	**5.00**	**3.14**	**2.98**	**2.84**	**2.67**	**2.58**	**2.59**	**2.57**
Y3-methyl-5-isopropylphenol	1.68	1.65	1.74	1.75	1.88	2.10	1.04	0.76	0.71	0.51	0.45	0.42	0.42
S4-isopropyl-3-methylphenol	**5.41**	**9.61**	**11.64**	**10.42**	**15.15**	**13.31**	**18.04**	**18.11**	**18.19**	**17.06**	**16.98**	**16.78**	**16.98**
Y3-methyl-4-isopropylphenol	1.51	3.09	4.53	5.35	6.91	5.60	5.94	4.61	4.56	3.24	2.94	2.72	2.81
S2-isopropyl-3-methylphenol	**0.63**	**1.46**	**2.29**	**2.04**	**3.04**	**2.31**	**5.89**	**6.78**	**7.09**	**7.86**	**8.20**	**8.38**	**8.45**
Y3-methyl-2-isopropylphenol	0.18	0.47	0.89	1.05	1.39	0.97	1.94	1.72	1.78	1.49	1.42	1.36	1.40
Thymol	66.62	72.06	73.47	73.32	72.29	72.75	68.69	68.11	67.76	68.04	67.66	67.74	67.51
3-methyl-5-isopropylphenol	16.69	8.86	6.43	5.73	5.11	6.61	3.64	3.41	3.25	3.10	3.00	3.01	2.98
3-methyl-2-isopropylphenol	14.96	16.57	16.79	17.51	18.81	17.59	20.86	20.73	20.86	19.76	19.78	19.50	19.70
3-methyl-4-isopropylphenol	1.74	2.51	3.31	3.43	3.78	3.05	6.81	7.75	8.13	9.10	9.56	9.75	9.81
STotal.Isomer	**36.19**	**57.97**	**69.33**	**59.52**	**80.52**	**75.64**	**86.47**	**87.40**	**87.20**	**86.37**	**85.82**	**86.04**	**86.18**
YTotal.Isomer	10.09	18.63	27.00	30.55	36.71	31.82	28.48	22.23	21.87	16.42	14.88	13.94	14.25
Slights	6.39	2.36	2.01	1.13	1.19	1.46	0.97	1.02	1.09	1.14	1.21	1.15	1.17
Ylights	1.78	0.76	0.78	0.58	0.54	0.62	0.32	0.26	0.27	0.22	0.21	0.19	0.19
SC-10	19.49	16.46	12.28	7.73	8.18	9.38	5.02	4.64	4.31	4.34	4.11	4.09	4.06
YC-10	5.43	5.29	4.78	3.97	3.73	3.95	1.65	1.18	1.08	0.83	0.71	0.66	0.67
Sdi-isopropylated	7.44	6.59	5.47	4.14	4.31	5.04	2.65	2.03	2.07	1.70	1.62	1.52	1.54
Ydi-isopropylated	2.08	2.12	2.13	2.13	1.96	2.12	0.87	0.52	0.52	0.32	0.28	0.25	0.26
Sheavies	13.24	10.73	7.01	25.91	3.20	5.56	1.39	0.76	0.86	0.75	0.99	0.65	0.55
Yheavies	3.69	3.45	2.73	13.30	1.46	2.34	0.46	0.19	0.22	0.14	0.17	0.11	0.09
Sether	0.92	0.20	0.34	0.23	0.15	0.23	0.65	1.01	1.04	1.51	1.73	1.83	1.86
Yether	0.26	0.06	0.13	0.12	0.07	0.10	0.21	0.26	0.26	0.29	0.30	0.30	0.31

Table 0.32: Conversion, selectivity and yield data for H-MFI-90 powder

	PW-35	PW-36	PW-37	PW-38	PW2-40	PW-41	PW-42	PW-43	PW-44	PW-45	PW-46
Time on Stream	92:01:00	93:01:00	94:01:00	95:01:00	97:01:00	98:01:00	103:01:00	103:31:00	104:01:00	104:31:00	105:01:00
Entry Temperature	88	88	88	88	88	88	83	83	84	84	84
Temperature	275	275	275	275	275	274	275	274	274	275	275
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	1.81	1.81	1.81	1.81	1.81
Pump Rate (ml/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.302	0.302	0.302	0.302	0.302
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3
Conversion	15.08	14.59	14.06	13.87	13.98	13.74	7.11	6.64	6.68	6.43	6.36
Thymol Selectivity	57.38	57.34	57.02	57.16	56.92	57.24	50.42	49.78	49.93	49.79	49.88
Thymol Yield	8.65	8.36	8.02	7.93	7.96	7.87	3.58	3.30	3.34	3.20	3.17
S3-isopropyl-5-methylphenol	**2.55**	**2.52**	**2.51**	**2.53**	**2.54**	**2.54**	**2.23**	**2.24**	**2.23**	**2.22**	**2.21**
Y3-methyl-5-isopropylphenol	0.38	0.37	0.35	0.35	0.36	0.35	0.16	0.15	0.15	0.14	0.14
S4-isopropyl-3-methylphenol	**16.70**	**16.72**	**16.30**	**16.61**	**16.50**	**16.31**	**15.34**	**15.22**	**15.56**	**15.38**	**15.40**
Y3-methyl-4-isopropylphenol	2.52	2.44	2.29	2.30	2.31	2.24	1.09	1.01	1.04	0.99	0.98
S2-isopropyl-3-methylphenol	**8.95**	**8.86**	**8.97**	**8.90**	**8.89**	**8.99**	**9.49**	**9.50**	**9.58**	**9.44**	**9.51**
Y3-methyl-2-isopropylphenol	1.35	1.29	1.26	1.23	1.24	1.24	0.67	0.63	0.64	0.61	0.60
Thymol	67.05	67.12	67.25	67.09	67.08	67.28	65.08	64.87	64.59	64.81	64.78
3-methyl-5-isopropylphenol	2.97	2.95	2.95	2.97	2.99	2.99	2.88	2.92	2.89	2.89	2.88
3-methyl-2-isopropylphenol	19.51	19.57	19.22	19.49	19.44	19.17	19.80	19.83	20.13	20.01	19.99
3-methyl-4-isopropylphenol	10.46	10.37	10.58	10.45	10.48	10.57	12.25	12.38	12.39	12.29	12.35
STotal.Isomer	**85.57**	**85.43**	**84.80**	**85.21**	**84.85**	**85.08**	**77.48**	**76.74**	**77.30**	**76.82**	**77.00**
YTotal.Isomer	12.90	12.46	11.93	11.82	11.86	11.69	5.51	5.09	5.17	4.94	4.90
Slights	1.02	1.18	1.21	1.15	1.32	1.21	1.58	1.61	1.47	1.64	1.65
Ylights	0.15	0.17	0.17	0.16	0.18	0.17	0.11	0.11	0.10	0.11	0.10
SC-10	3.88	3.86	3.85	3.85	3.86	3.82	3.15	3.13	3.08	3.09	3.09
YC-10	0.58	0.56	0.54	0.53	0.54	0.52	0.22	0.21	0.21	0.20	0.20
Sdi-isopropylated	1.49	1.42	1.43	1.41	1.40	1.38	0.77	0.87	0.91	0.80	0.82
Ydi-isopropylated	0.22	0.21	0.20	0.20	0.20	0.19	0.05	0.06	0.06	0.05	0.05
Sheavies	0.69	0.66	0.87	0.64	0.80	0.54	1.81	1.65	1.07	1.17	0.72
Yheavies	0.10	0.10	0.12	0.09	0.11	0.07	0.13	0.11	0.07	0.07	0.05
Sether	2.33	2.26	2.44	2.33	2.37	2.50	5.34	5.42	5.74	5.66	5.78
Yether	0.35	0.33	0.34	0.32	0.33	0.34	0.38	0.36	0.38	0.36	0.37

Table 0.33: Conversion, selectivity and yield data for H-MFI-90 powder (cont.)

	PW-47	PW-48	PW-49	PW-50	PW-51	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59
Time on Stream	116:31:00	117:01:00	117:31:00	118:01:00	127:01:00	135:01:00	137:01:00	139:01:00	141:01:00	141:31:00	180:53:22	188:56:55	190:00:55
Entry Temperature	87	85	85	85	88	86	86	86	86	86	86	89	90
Temperature	274	274	275	275	275	275	274	275	275	275	275	276	276
WHSV	3.62	3.62	3.62	3.62	3.62	0.3	0.3	0.3	0.3	0.3	0.96	0.96	0.96
Pump Rate (ml/min)	0.6042	0.604	0.604	0.604	0.604	0.05	0.05	0.05	0.05	0.05	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	2.00	1.88	1.83	1.71	1.98	26.62	26.28	24.58	27.10	26.94	12.15	11.04	9.31
Thymol Selectivity	23.39	20.73	19.40	17.72	21.73	63.44	62.43	62.69	62.01	62.65	56.25	56.25	56.57
Thymol Yield	0.47	0.39	0.35	0.30	0.43	16.89	16.40	15.41	16.80	16.88	6.83	6.21	5.27
S3-isopropyl-5-methylphenol	**1.23**	**1.00**	**1.02**	**0.90**	**1.13**	**2.86**	**2.92**	**2.99**	**3.00**	**2.81**	**2.61**	**2.43**	**2.30**
Y3-methyl-5-isopropylphenol	0.02	0.02	0.02	0.02	0.02	0.76	0.77	0.74	0.81	0.76	0.32	0.27	0.21
S4-isopropyl-3-methylphenol	**8.46**	**7.36**	**6.65**	**6.16**	**6.75**	**13.40**	**13.81**	**13.71**	**13.82**	**13.96**	**15.40**	**14.97**	**14.53**
Y3-methyl-4-isopropylphenol	0.17	0.14	0.12	0.11	0.13	3.57	3.63	3.37	3.75	3.76	1.87	1.65	1.35
S2-isopropyl-3-methylphenol	**5.55**	**5.24**	**4.80**	**4.84**	**5.77**	**6.74**	**6.79**	**6.45**	**6.69**	**6.78**	**9.10**	**9.70**	**9.49**
Y3-methyl-2-isopropylphenol	0.11	0.10	0.09	0.08	0.11	1.80	1.79	1.58	1.81	1.83	1.10	1.07	0.88
Thymol	60.56	60.38	60.87	59.83	61.42	73.40	72.63	73.03	72.50	72.68	67.48	67.48	68.25
3-methyl-5-isopropylphenol	3.18	2.92	3.19	3.03	3.20	3.31	3.40	3.49	3.51	3.26	3.13	2.92	2.78
3-methyl-2-isopropylphenol	21.90	21.44	20.87	20.81	19.08	15.50	16.07	15.97	16.16	16.20	18.48	17.96	17.53
3-methyl-4-isopropylphenol	14.36	15.26	15.07	16.33	16.30	7.80	7.90	7.51	7.83	7.87	10.91	11.64	11.45
STotal.Isomer	**38.63**	**34.33**	**31.87**	**29.62**	**35.38**	**86.44**	**85.96**	**85.84**	**85.52**	**86.21**	**83.36**	**83.37**	**82.90**
YTotal.Isomer	0.77	0.64	0.58	0.51	0.70	23.01	22.59	21.10	23.17	23.23	10.13	9.20	7.72
Slights	4.25	4.17	4.95	4.88	4.13	1.09	1.20	1.19	1.18	1.21	1.44	1.34	1.05
Ylights	0.08	0.08	0.09	0.08	0.08	0.29	0.32	0.29	0.32	0.33	0.18	0.15	0.10
SC-10	1.08	0.92	0.65	0.51	1.28	4.84	4.85	4.94	4.90	4.77	4.14	3.99	3.94
YC-10	0.02	0.02	0.01	0.01	0.03	1.29	1.27	1.21	1.33	1.28	0.50	0.44	0.37
Sdi-isopropylated	0.17	0.29	0.39	0.39	0.45	2.46	2.61	2.77	2.87	2.56	1.79	1.38	1.17
Ydi-isopropylated	0.00	0.01	0.01	0.01	0.01	0.65	0.69	0.68	0.78	0.69	0.22	0.15	0.11
Sheavies	1.57	3.66	4.18	5.05	8.02	0.82	1.03	0.78	1.21	1.05	0.82	0.85	0.63
Yheavies	0.03	0.07	0.08	0.09	0.16	0.22	0.27	0.19	0.33	0.28	0.10	0.09	0.06
Sether	20.22	20.66	20.73	19.25	16.39	0.76	0.75	0.74	0.73	0.71	2.26	2.45	2.57
Yether	0.40	0.39	0.38	0.33	0.32	0.20	0.20	0.18	0.20	0.19	0.27	0.27	0.24

Table 0.34: GC raw data for microchannel reactor

		MR-1	MR-2	MR-3	MR-4	MR-5	MR-6	MR-7	MR-8	MR-9	MR-10
Time on Stream		2:42:36	42:14:51	59:07:27	65:04:27	75:09:27	88:56:27	99:05:27	113:01:27	123:12:27	135:38:27
		275	275	275	276	276	275	275	275	275	276
Entry Temperature		77	75	75	77	77	77	77	77	77	76
WHSV		1.85	1.85	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
		0.001	0.001	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
		2	2	2	2	2	2	3	3	2	2
Isopropyl-Tolyl Ether	± 4.70	23.8	2.2	1	2.8	3.7	3.6	5.3	4.1	4.8	10.4
???	± 5.04		1	2.1	0.9	1	1.3	2.1	1.8	1.6	1.8
phenol	± 5.26		12.9								1.2
o-cresol	± 5.35	11.1	8.4	12.2	8.7	8.7	5.4	7.7	4.9	4.2	17.4
p-Cresol	± 5.60	70	42.9	63.5	59.6	70.9	45.9	69.3	50.3	46.1	160.9
m-Cresol	± 5.80	10232.9	5043.2	6146	7689.5	9945.2	6398.1	10295.2	7528.4	7052.9	24387.1
???	± 6.00	7	3.8	4.2	5.1	5.7	3.9	5.5	4.6	4.3	14.3
2,4-Xylenol	± 6.20	2.7	2.7	2.6	2	1.9	1.3	1.6	1.7	0.5	3.6
2,5-Xylenol	± 6.50	3.7	1.9	1.9	2.8	3.3	2.1	3.5	2.3	2.1	8.4
2,3-Xylenol	± 6.74										
???	± 6.90										
???	± 7.03		1.4	1.8	1.6						
???	± 7.16	1.5	1.6	2.4	1.5	1.2	1.5	1	0.6	0.3	1.7
2-Isopropyl-4-methyl Phenol	± 7.30	5.9	1.5	1.6				0.5	2.1	0.6	1.8
???	± 7.49										
Thymol isomer (2,3)	± 7.60	78.6	3.9	4.4	5.9	7.6	9.3	11	14.8	11.1	32.6
???	± 7.73	2.4	2.3	7	4	2.9	3.3	2.2	2.2	1.3	6.3
Thymol	± 7.90	454.6	57	74.7	69.9	70	73.2	79.7	109.2	66.8	192.7
????	± 8.19	2	2.6	6.7	3.8	2.8	2.3	1.8	2.4	1.3	4.7
????	± 8.33	25.1	38.1	66.5	48.9	41	36.4	32.8	28.4	14.4	49.8
6-n-Propyl-3-Methyl Phenol	± 8.40	8.1									
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	3.5	6.2	14.9	9.3	6.7	6.1	4.8	4.1	1.8	6.8
5,3 Thymol Isomer	± 8.67	23.6	2.2	3.9	3.1	2.8	3	3.4	5.1	3.6	11.9
4,3 Thymol isomer	± 8.78	80.9	3.8	5.2	5.3	5.5	6	7.1	11.3	8.4	23.9
C-13 fraction (13.02)	± 8.83		0.5	0.9							
????	± 9.22	2.1	2.6	2.8	3.2	2.5	3.3	2.2	3	2	4.9
????	± 9.48	1.8	0.6	3	0.9	2.4	1.3	1.5	0.7	1.4	2
????	± 9.60										
????	± 10.30	1.1	4.5	9.2	4.1	3.5	3.7	2	2	0.9	6.1
????	± 10.70		0.9	1.9	1.3	1					
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	31.7						1.3	2.9	2.1	3.2
????	± 11.30										
????	± 11.56										
????	± 11.87										
(15.72,15.88)	± 12.21										
5,6-Diisopropyl-3-Methyl Phenol	± 12.70	2.3									
Heavies	± 13.04		2.6	2.4	1.3	1.9	2	0.7			1.6
Heavies		9.6	12.6	14.3	11.8	14.9	9.6	11.5	11.8	11	16.3

Table 0.35: GC raw data for microchannel reactor (cont.)

		MR-11	MR-12	MR-13	MR-14	MR-15	MR-16	MR-17	MR-18	MR-19	MR-20
Time on Stream		145:14:27	157:10:27	169:09:27	180:42:28	191:59:37	204:16:37	216:04:37	228:08:37	261:10:37	271:52:37
Temperature		300	300	300	300	300	300	300	300	300	325
Entry Temperature		76	74	70	74	73	73	73	74	74	73
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	5.6	5.1	9.2	17.4	32.8	26.7	17.6	12.7	13.9	5
???	± 5.04	1.8	1.7	0.7	2.1	1					
phenol	± 5.26	1	1.2	1	1.2	1.7	4.5	0.8	0.4		
o-cresol	± 5.35	10.4	8.7	3.6	5.1	7.6	5.2	2.6	3.5	8.2	3.4
p-Cresol	± 5.60	89.9	74	37.9	54.3	75	55.5	35.3	35.9	72.9	35.4
m-Cresol	± 5.80	12104.3	9620.7	5518.7	8335.5	11830.8	8716.2	5354.7	5096.3	10910.8	5188
???	± 6.00	6.7	5.8	3.5	4.2	7.3	5.6	3.4	3.1	6.2	3.1
2,4-Xylenol	± 6.20	2.4	1.6	1.2	1.5	1.8	0.9	0.8	2.4	1.6	1
2,5-Xylenol	± 6.50	4.2	3.6	1.9	3	4.2	2.9	1.7	2.2	3.7	1.5
2,3-Xylenol	± 6.74		1								
???	± 6.90										
???	± 7.03		1.4								
???	± 7.16	2.4	2.5	1.2	0.5	1.1	0.5	0.5	1.4		
2-Isopropyl-4-methyl Phenol	± 7.30	1.2	2.1	1.7	3.6	5.5	2.5	1.8	2.3		
???	± 7.49										
Thymol isomer (2,3)	± 7.60	19.4	23.3	31.6	67.7	120.2	64.7	27.7	25.3	12.7	7.5
???	± 7.73	6.5	8.5	2	3.2	2.6	1.2	0.8	1.3		
Thymol	± 7.90	152	189.2	153.2	320.7	513.4	243.3	135.1	182.8	48.1	33.4
????	± 8.19	5.5	5.9	1.8	2.3	2.5	1.1	1.1	1.1		
????	± 8.33	86.1	108.6	29.7	23.9	20.7	7.7	8.3	16.1	5.8	5
6-n-Propyl-3-Methyl Phenol	± 8.40			1.4	4.6	9.5	4.2	1.7	1.4		
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	10.9	14.6	3.3	2.7	1.7	1.1	0.7	1.4		
5,3 Thymol Isomer	± 8.67	7.7	9.8	7.4	16.2	28.1	12.9	13.4	22.9	4.6	3.7
4,3 Thymol isomer	± 8.78	16	21.2	21.5	49.1	79.6	68.1	20.9	28.4	8.3	5.8
C-13 fraction (13.02)	± 8.83										
????	± 9.22	3.6	4.6	2.2	2.8	4.6	1.2	1.8	3.6		
????	± 9.48	1.5	2	2	2.2	2					
????	± 9.60										
????	± 10.30	5.1	7.1	1.1	0.7	0.8					
????	± 10.70	1.5	1.2			2.8					
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	3.3	2.8	5.2	16	31	13.6	6.8	8.5	1.3	1.4
????	± 11.30										
????	± 11.56										
????	± 11.87										
(15.72,15.88)	± 12.21										
5,6-Diisopropyl-3-Methyl Phenol	± 12.70										
Heavies	± 13.04	2	3								
Heavies		11.7	18.6	29.9	15.8	13.7	18.9	14.9	10.5	14.5	19

Table 0.36: GC raw data for microchannel reactor (cont.)

		MR-21	MR-22	MR-23	MR-24	MR-25	MR-26	MR-27	MR-28	MR-29	MR-30
Time on Stream		281:34:37	309:39:37	319:52:37	342:40:37	353:19:37	364:28:37	375:51:37	388:30:37	442:02:37	449:27:37
Temperature		325	325	325	325	325	325	325	325	325	325
Entry Temperature		64	74	73	77	77	77	78	77	77	77
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	12.7	7.6	3.3	1.5	2.2	2.3	2.7	4.4	6.7	5.2
???	± 5.04	2.3			0.4	0.7					
phenol	± 5.26										
o-cresol	± 5.35	5.3	5	1.8	3.6	6.3	4.8	6	5.8	9	7
p-Cresol	± 5.60	56.8	53.3	27.1	44	71	60.9	58.8	62.8	90.2	73.4
m-Cresol	± 5.80	8870	8313.2	4293.6	6704.3	11219.4	9571.8	9299.7	10018.7	14397.2	11743.2
???	± 6.00	4.8	4.7	2	3.5	6.2	5.4	4.9	5.6	8.6	6
2,4-Xylenol	± 6.20	1.5	1.1	1.6	1.9	1.7	1.4	1.1	1.3	1.2	1.1
2,5-Xylenol	± 6.50	2.9	3	2.2	2.4	4	3.7	2.9	3.1	4.9	3.7
2,3-Xylenol	± 6.74										
???	± 6.90										
???	± 7.03										
???	± 7.16										
2-Isopropyl-4-methyl Phenol	± 7.30										
???	± 7.49										
Thymol isomer (2,3)	± 7.60	11.5	7.4	3.5	5.2	4.4	3.1	2.9	5.2	7.3	7.4
???	± 7.73					2		2.3			
Thymol	± 7.90	46.4	33	13.5	47.8	32.5	18.2	9.9	20.1	22.3	25.8
????	± 8.19										
????	± 8.33	2.7	1.6	1.2	3.5	2.3	1.3	0.3	0.3		
6-n-Propyl-3-Methyl Phenol	± 8.40										
2,6-Diisopropyl-3-Methyl Phenol	± 8.55										
5,3 Thymol Isomer	± 8.67	4.8	3.9	1.6	10.1	7.3	3.5	1.4	1.2	1	1.8
4,3 Thymol isomer	± 8.78	9.1	7	3.2	8.4	6.4	3.4	1.5	3.9	4.1	5.4
C-13 fraction (13.02)	± 8.83										
????	± 9.22										
????	± 9.48										
????	± 9.60										
????	± 10.30										
????	± 10.70										
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	3.6	0.9								
????	± 11.30										
????	± 11.56										
????	± 11.87										
(15.72,15.88)	± 12.21										
5,6-Diisopropyl-3-Methyl Phenol	± 12.70										
Heavies	± 13.04										
Heavies		20.4	20.1	20.5	23.9	10.2	10.2	11.1	9.6	14	13

Table 0.37: GC raw data for microchannel reactor (cont.)

		MR-31	MR-32	MR-33	MR-34	MR-35	MR-36	MR-37
Time on Stream		451:02:37	457:30:37	463:20:37	475:24:37	480:11:37	489:30:37	499:54:37
Temperature		275	275	274	275	275	274	275
Entry Temperature		76	74	76	76	77	78	78
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	4.8	8.4	12	24	42.3	20.4	22.6
???	± 5.04							
phenol	± 5.26							
o-cresol	± 5.35	6.2	8.5	3.8	5	4.9	2.9	2.4
p-Cresol	± 5.60	65.1	69.3	41.7	57.5	63.8	33.1	29.9
m-Cresol	± 5.80	10348.1	11005.9	6516.9	9114.5	10056.5	5155	4688.5
???	± 6.00	5.1	6.1	4	5.2	4.5	3.3	2.8
2,4-Xylenol	± 6.20	0.9	0.8	0.7	0.8	1.1	0.7	0.9
2,5-Xylenol	± 6.50	3.6	4.1	2.1	3.4	3.2	1.5	1.8
2,3-Xylenol	± 6.74							
???	± 6.90							
???	± 7.03							
???	± 7.16							
2-Isopropyl-4-methyl Phenol	± 7.30				0.7			
???	± 7.49							
Thymol isomer (2,3)	± 7.60	4.5	8.1	13.8	24.8	28.2	13.4	15.3
???	± 7.73							
Thymol	± 7.90	14.6	23.6	42	75.8	70.9	36.4	35.9
????	± 8.19							
????	± 8.33			0.7	0.9	0.9	1.1	
6-n-Propyl-3-Methyl Phenol	± 8.40				1.2	1.8	0.4	0.7
2,6-Diisopropyl-3-Methyl Phenol	± 8.55							
5,3 Thymol Isomer	± 8.67	0.9	1.6	2.2	3.7	2.6	2.7	1.5
4,3 Thymol isomer	± 8.78	3	5.2	7.6	13.8	13.1	8.3	7.6
C-13 fraction (13.02)	± 8.83							
????	± 9.22							
????	± 9.48							
????	± 9.60							
????	± 10.30							
????	± 10.70							
4,6-Diisopropyl-3-Methyl Phenol	± 11.18			1.9	4.3	3.9	3	2.8
????	± 11.30							
????	± 11.56							
????	± 11.87							
(15.72,15.88)	± 12.21							
5,6-Diisopropyl-3-Methyl Phenol	± 12.70							
Heavies	± 13.04							
Heavies		14.6	12.2	12.9	11.4	12.3	11.6	11.9

Table 0.38: Product composition (%) for microchannel reactor

		MR-1	MR-2	MR-3	MR-4	MR-5	MR-6	MR-7	MR-8	MR-9	MR-10
Time on Stream		2:42:36	42:14:51	59:07:27	65:04:27	75:09:27	88:56:27	99:05:27	113:01:27	123:12:27	135:38:27
Temperature		275	275	275	276	276	275	275	275	275	276
Entry Temperature		77	75	75	77	77	77	77	77	77	76
WHSV		1.85	1.85	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.001	0.001	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	3	3	2	2
Isopropyl-Tolyl Ether	± 4.70	0.16	0.03	0.01	0.03	0.03	0.04	0.04	0.04	0.05	0.03
???	± 5.04	-	0.02	0.03	0.01	0.01	0.02	0.02	0.02	0.02	0.01
phenol	± 5.26	-	0.18	-	-	-	-	-	-	-	0.00
o-cresol	± 5.35	0.10	0.16	0.19	0.11	0.09	0.08	0.07	0.06	0.06	0.07
p-Cresol	± 5.60	0.65	0.82	1.00	0.76	0.70	0.70	0.66	0.65	0.64	0.65
m-Cresol	± 5.80	94.54	96.84	96.35	97.53	98.02	97.46	98.10	97.42	98.01	98.19
???	± 6.00	0.05	0.06	0.05	0.05	0.04	0.05	0.04	0.05	0.05	0.04
2,4-Xylenol	± 6.20	0.02	0.04	0.03	0.02	0.01	0.02	0.01	0.02	0.01	0.01
2,5-Xylenol	± 6.50	0.03	0.03	0.02	0.03	0.02	0.02	0.03	0.02	0.02	0.03
2,3-Xylenol	± 6.74	-	-	-	-	-	-	-	-	-	-
???	± 6.90	-	0.02	0.02	0.02	-	-	-	-	-	-
???	± 7.03										
???	± 7.16	0.01	0.02	0.03	0.01	0.01	0.02	0.01	0.01	0.00	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.04	0.02	0.02	-	-	-	0.00	0.02	0.01	0.01
???	± 7.49	-	-	-	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	0.50	0.05	0.05	0.05	0.05	0.10	0.07	0.13	0.11	0.09
???	± 7.73	0.02	0.03	0.08	0.03	0.02	0.03	0.01	0.02	0.01	0.02
Thymol	± 7.90	2.88	0.75	0.80	0.61	0.47	0.76	0.52	0.97	0.64	0.53
????	± 8.19	0.01	0.03	0.07	0.03	0.02	0.02	0.01	0.02	0.01	0.01
????	± 8.33	0.16	0.50	0.72	0.43	0.28	0.38	0.21	0.25	0.14	0.14
6-n-Propyl-3-Methyl Phenol	± 8.40	0.04	-	-	-	-	-	-	-	-	-
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	0.02	0.08	0.16	0.08	0.05	0.06	0.03	0.04	0.02	0.02
5,3 Thymol Isomer	± 8.67	0.15	0.03	0.04	0.03	0.02	0.03	0.02	0.05	0.03	0.03
4,3 Thymol isomer	± 8.78	0.39	0.04	0.04	0.04	0.03	0.05	0.04	0.08	0.06	0.05
C-13 fraction (13.02)	± 8.83	-	0.01	0.01	-	-	-	-	-	-	-
????	± 9.22	0.01	0.03	0.02	0.02	0.01	0.03	0.01	0.02	0.01	0.01
????	± 9.48	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.00	0.00	0.00
????	± 9.60										
????	± 10.30	0.01	0.05	0.08	0.03	0.02	0.03	0.01	0.01	0.01	0.01
????	± 10.70	-	0.01	0.02	0.01	0.01	-	-	-	-	-
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	0.15	-	-	-	-	-	0.01	0.02	0.02	0.01
????	± 11.30	-	-	-	-	-	-	-	-	-	-
????	± 11.56	-	-	-	-	-	-	-	-	-	-
????	± 11.87	-	-	-	-	-	-	-	-	-	-
(15.72,15.88)	± 12.21	-	-	-	-	-	-	-	-	-	-
5,6-Diisopropyl-3-Methyl Phenol	± 12.70	0.01	-	-	-	-	-	-	-	-	-
Heavies	± 13.04	-	0.03	0.02	0.01	0.01	0.02	0.00	-	-	0.00
Heavies		0.05	0.13	0.12	0.08	0.08	0.08	0.06	0.08	0.08	0.03

Table 0.39: Product composition (%) for microchannel reactor (cont.)

		MR-11	MR-12	MR-13	MR-14	MR-15	MR-16	MR-17	MR-18	MR-19	MR-20
Time on Stream		145:14:27	157:10:27	169:09:27	180:42:28	191:59:37	204:16:37	216:04:37	228:08:37	261:10:37	271:52:37
Temperature		300	300	300	300	300	300	300	300	325	325
Entry Temperature		76	74	70	74	73	73	73	74	74	73
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	0.03	0.04	0.11	0.14	0.19	0.21	0.23	0.17	0.09	0.07
???	± 5.04	0.01	0.02	0.01	0.02	0.01	-	-	-	-	-
phenol	± 5.26	0.01	0.01	0.01	0.01	0.01	0.04	0.01	0.01	-	-
o-cresol	± 5.35	0.08	0.09	0.06	0.06	0.06	0.06	0.05	0.07	0.07	0.06
p-Cresol	± 5.60	0.72	0.74	0.66	0.62	0.60	0.61	0.63	0.67	0.66	0.67
m-Cresol	± 5.80	97.26	96.19	95.72	95.07	94.63	95.87	96.23	95.20	98.54	98.21
???	± 6.00	0.04	0.04	0.05	0.04	0.04	0.05	0.05	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.03	0.01	0.01
2,5-Xylenol	± 6.50	0.03	0.03	0.03	0.03	0.03	0.02	0.02	0.03	0.03	0.02
2,3-Xylenol	± 6.74	-	0.01	-	-	-	-	-	-	-	-
???	± 6.90	-	0.01	-	-	-	-	-	-	-	-
???	± 7.03										
???	± 7.16	0.01	0.02	0.02	0.00	0.01	0.00	0.01	0.02	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	0.01	0.02	0.02	0.03	0.03	0.02	0.02	0.03	-	-
???	± 7.49	-	-	-	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	0.11	0.16	0.38	0.53	0.66	0.49	0.34	0.32	0.08	0.10
???	± 7.73	0.04	0.06	0.02	0.03	0.01	0.01	0.01	0.02	-	-
Thymol	± 7.90	0.84	1.30	1.82	2.51	2.82	1.84	1.67	2.34	0.30	0.43
????	± 8.19	0.03	0.04	0.02	0.02	0.01	0.01	0.01	0.01	-	-
????	± 8.33	0.47	0.74	0.35	0.19	0.11	0.06	0.10	0.21	0.04	0.06
6-n-Propyl-3-Methyl Phenol	± 8.40	-	-	0.01	0.03	0.04	0.02	0.02	0.01	-	-
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	0.06	0.10	0.04	0.02	0.01	0.01	0.01	0.02	-	-
5,3 Thymol Isomer	± 8.67	0.04	0.07	0.09	0.13	0.15	0.10	0.17	0.29	0.03	0.05
4,3 Thymol isomer	± 8.78	0.07	0.11	0.19	0.29	0.33	0.39	0.20	0.28	0.04	0.06
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-
????	± 9.22	0.02	0.02	0.02	0.02	0.02	0.01	0.02	0.04	-	-
????	± 9.48	0.01	0.01	0.02	0.01	0.01	-	-	-	-	-
????	± 9.60										
????	± 10.30	0.02	0.04	0.01	0.00	0.00	-	-	-	-	-
????	± 10.70	0.01	0.01	-	-	0.01	-	-	-	-	-
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	0.01	0.01	0.05	0.10	0.13	0.08	0.06	0.08	0.01	0.01
????	± 11.30	-	-	-	-	-	-	-	-	-	-
????	± 11.56	-	-	-	-	-	-	-	-	-	-
????	± 11.87	-	-	-	-	-	-	-	-	-	-
(15.72,15.88)	± 12.21	-	-	-	-	-	-	-	-	-	-
5,6-Diisopropyl-3-Methyl Phenol	± 12.70	-	-	-	-	-	-	-	-	-	-
Heavies	± 13.04	0.01	0.02	-	-	-	-	-	-	-	-
Heavies		0.05	0.10	0.27	0.09	0.06	0.11	0.14	0.10	0.07	0.19

Table 0.40: Product composition (%) for microchannel reactor (cont.)

		MR-21	MR-22	MR-23	MR-24	MR-25	MR-26	MR-27	MR-28	MR-29	MR-30
Time on Stream		281:34:37	309:39:37	319:52:37	342:40:37	353:19:37	364:28:37	375:51:37	388:30:37	442:02:37	449:27:37
Temperature		325	325	325	325	325	325	325	325	325	325
Entry Temperature		64	74	73	77	77	77	78	77	77	77
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	0.10	0.06	0.05	0.02	0.01	0.02	0.02	0.03	0.03	0.03
???	± 5.04	0.03	-	-	0.01	0.01	-	-	-	-	-
phenol	± 5.26	-	-	-	-	-	-	-	-	-	-
o-cresol	± 5.35	0.06	0.06	0.04	0.05	0.06	0.05	0.06	0.06	0.06	0.06
p-Cresol	± 5.60	0.63	0.63	0.62	0.64	0.63	0.63	0.63	0.62	0.62	0.62
m-Cresol	± 5.80	98.42	98.62	98.58	98.28	98.85	98.96	99.02	98.96	99.00	98.94
???	± 6.00	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.03	0.02	0.01	0.01	0.01	0.01	0.01	0.01
2,5-Xylenol	± 6.50	0.02	0.03	0.04	0.03	0.03	0.03	0.02	0.02	0.03	0.02
2,3-Xylenol	± 6.74	-	-	-	-	-	-	-	-	-	-
???	± 6.90	-	-	-	-	-	-	-	-	-	-
???	± 7.03										
???	± 7.16	-	-	-	-	-	-	-	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	-	-	-	-	-	-	-	-	-	-
???	± 7.49	-	-	-	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	0.09	0.06	0.06	0.05	0.03	0.02	0.02	0.04	0.03	0.04
???	± 7.73	-	-	-	-	0.01	-	0.02	-	-	-
Thymol	± 7.90	0.35	0.27	0.21	0.48	0.20	0.13	0.07	0.14	0.11	0.15
????	± 8.19	-	-	-	-	-	-	-	-	-	-
????	± 8.33	0.02	0.01	0.02	0.04	0.01	0.01	0.00	0.00	-	-
6-n-Propyl-3-Methyl Phenol	± 8.40	-	-	-	-	-	-	-	-	-	-
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	-	-	-	-	-	-	-	-	-	-
5,3 Thymol Isomer	± 8.67	0.04	0.03	0.03	0.10	0.04	0.02	0.01	0.01	0.00	0.01
4,3 Thymol isomer	± 8.78	0.05	0.04	0.04	0.06	0.03	0.02	0.01	0.02	0.01	0.02
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-
????	± 9.22	-	-	-	-	-	-	-	-	-	-
????	± 9.48	-	-	-	-	-	-	-	-	-	-
????	± 9.60										
????	± 10.30	-	-	-	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	0.02	0.01	-	-	-	-	-	-	-	-
????	± 11.30	-	-	-	-	-	-	-	-	-	-
????	± 11.56	-	-	-	-	-	-	-	-	-	-
????	± 11.87	-	-	-	-	-	-	-	-	-	-
(15.72,15.88)	± 12.21	-	-	-	-	-	-	-	-	-	-
5,6-Diisopropyl-3-Methyl Phenol	± 12.70	-	-	-	-	-	-	-	-	-	-
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-
Heavies		0.12	0.12	0.25	0.18	0.05	0.06	0.06	0.05	0.05	0.06

Table 0.41: Product composition (%) for microchannel reactor (cont.)

		MR-31	MR-32	MR-33	MR-34	MR-35	MR-36	MR-37
Time on Stream		451:02:37	457:30:37	463:20:37	475:24:37	480:11:37	489:30:37	499:54:37
Temperature		275	275	274	275	275	274	275
Entry Temperature		76	74	76	76	77	78	78
WHSV		3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)		0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)		2	2	2	2	2	2	2
Isopropyl-Tolyl Ether	± 4.70	0.03	0.05	0.13	0.19	0.30	0.28	0.34
???	± 5.04	-	-	-	-	-	-	-
phenol	± 5.26	-	-	-	-	-	-	-
o-cresol	± 5.35	0.06	0.08	0.06	0.05	0.05	0.06	0.05
p-Cresol	± 5.60	0.62	0.62	0.63	0.62	0.62	0.63	0.62
m-Cresol	± 5.80	99.00	98.88	98.32	98.11	98.12	98.03	97.89
???	± 6.00	0.04	0.04	0.05	0.04	0.03	0.05	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.01	0.01	0.01
2,5-Xylenol	± 6.50	0.03	0.03	0.02	0.03	0.02	0.02	0.03
2,3-Xylenol	± 6.74	-	-	-	-	-	-	-
???	± 6.90	-	-	-	-	-	-	-
???	± 7.03							
???	± 7.16	-	-	-	-	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	-	-	-	0.01	-	-	-
???	± 7.49	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	0.03	0.05	0.14	0.18	0.19	0.17	0.22
???	± 7.73	-	-	-	-		-	-
Thymol	± 7.90	0.10	0.15	0.43	0.56	0.47	0.47	0.51
????	± 8.19	-	-	-	-	-	-	-
????	± 8.33	-	-	0.01	0.01	0.01	0.01	-
6-n-Propyl-3-Methyl Phenol	± 8.40	-	-	-	0.01	0.01	0.00	0.01
2,6-Diisopropyl-3-Methyl Phenol	± 8.55	-	-	-	-	-	-	-
5,3 Thymol Isomer	± 8.67	0.01	0.01	0.02	0.03	0.02	0.04	0.02
4,3 Thymol isomer	± 8.78	0.01	0.02	0.06	0.08	0.07	0.08	0.08
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-
????	± 9.22	-	-	-	-	-	-	-
????	± 9.48	-	-	-	-	-	-	-
????	± 9.60							
????	± 10.30	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-
4,6-Diisopropyl-3-Methyl Phenol	± 11.18	-	-	0.01	0.02	0.02	0.03	0.03
????	± 11.30	-	-	-	-	-	-	-
????	± 11.56	-	-	-	-	-	-	-
????	± 11.87	-	-	-	-	-	-	-
(15.72,15.88)	± 12.21	-	-	-	-	-	-	-
5,6-Diisopropyl-3-Methyl Phenol	± 12.70	-	-	-	-	-	-	-
Heavies	± 13.04	-	-	-	-	-	-	-
Heavies		0.07	0.06	0.10	0.06	0.06	0.12	0.13

Table 0.42: Conversion, selectivity and yield data for microchannel reactor

	MR-1	MR-2	MR-3	MR-4	MR-5	MR-6	MR-7	MR-8	MR-9	MR-10
Time on Stream	2:42:36	42:14:51	59:07:27	65:04:27	75:09:27	88:56:27	99:05:27	113:01:27	123:12:27	135:38:27
Temperature	275	275	275	276	276	275	275	275	275	276
Entry Temperature	77	75	75	77	77	77	77	77	77	76
WHSV	1.85	1.85	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.001	0.001	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	3	3	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	5.46	3.16	3.65	2.47	1.98	2.54	1.90	2.58	1.99	1.81
Thymol Selectivity	52.80	23.73	22.04	24.57	23.90	30.05	27.47	37.61	32.07	29.33
Thymol Yield	2.88	0.75	0.80	0.61	0.47	0.76	0.52	0.97	0.64	0.53
S3-isopropyl-5-methylphenol	**2.74**	**0.92**	**1.15**	**1.09**	**0.96**	**1.23**	**1.17**	**1.76**	**1.73**	**1.81**
Y3-methyl-5-isopropylphenol	0.15	0.03	0.04	0.03	0.02	0.03	0.02	0.05	0.03	0.03
S4-isopropyl-3-methylphenol	**7.15**	**1.20**	**1.17**	**1.42**	**1.43**	**1.87**	**1.86**	**2.96**	**3.07**	**2.77**
Y3-methyl-4-isopropylphenol	0.39	0.04	0.04	0.04	0.03	0.05	0.04	0.08	0.06	0.05
S2-isopropyl-3-methylphenol	**9.13**	**1.62**	**1.30**	**2.07**	**2.60**	**3.82**	**3.79**	**5.10**	**5.33**	**4.96**
Y3-methyl-2-isopropylphenol	0.50	0.05	0.05	0.05	0.05	0.10	0.07	0.13	0.11	0.09
Thymol	73.52	86.37	85.90	84.28	82.76	81.27	80.10	79.30	76.00	75.45
3-methyl-5-isopropylphenol	3.82	3.33	4.48	3.74	3.31	3.33	3.42	3.70	4.10	4.66
3-methyl-2-isopropylphenol	9.96	4.38	4.55	4.86	4.95	5.07	5.43	6.24	7.27	7.12
3-methyl-4-isopropylphenol	12.71	5.91	5.06	7.11	8.99	10.33	11.05	10.75	12.63	12.76
STotal.Isomer	**71.82**	**27.47**	**25.65**	**29.15**	**28.88**	**36.97**	**34.30**	**47.42**	**42.20**	**38.87**
YTotal.Isomer	3.92	0.87	0.94	0.72	0.57	0.94	0.65	1.22	0.84	0.71
Slights	2.70	6.00	4.78	5.10	4.62	4.03	4.66	4.35	4.18	5.07
Ylights	0.15	0.19	0.17	0.13	0.09	0.10	0.09	0.11	0.08	0.09
SC-10	3.43	17.90	23.66	19.93	15.95	17.24	12.68	11.37	8.16	9.25
YC-10	0.19	0.57	0.86	0.49	0.32	0.44	0.24	0.29	0.16	0.17
Sdi-isopropylated	0.92	1.11	0.97	0.70	0.75	0.62	0.18	-	-	0.19
Ydi-isopropylated	0.05	0.04	0.04	0.02	0.01	0.02	0.00	-	-	0.00
Sheavies	11.24	7.79	7.95	6.77	7.48	7.47	6.71	8.31	8.91	6.53
Yheavies	0.61	0.25	0.29	0.17	0.15	0.19	0.13	0.21	0.18	0.12
Sether	2.90	6.60	0.31	1.03	1.33	1.55	1.92	1.48	2.42	1.85

Table 0.43: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-11	MR-12	MR-13	MR-14	MR-15	MR-16	MR-17	MR-18	MR-19	MR-20
Time on Stream	145:14:27	157:10:27	169:09:27	180:42:28	191:59:37	204:16:37	216:04:37	228:08:37	261:10:37	271:52:37
Temperature	300	300	300	300	300	300	300	300	325	325
Entry Temperature	76	74	70	74	73	73	73	74	74	73
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	2.74	3.81	4.28	4.93	5.37	4.13	3.77	4.80	1.46	1.79
Thymol Selectivity	30.60	34.05	42.55	50.94	52.44	44.42	44.16	48.79	20.45	24.27
Thymol Yield	0.84	1.30	1.82	2.51	2.82	1.84	1.67	2.34	0.30	0.43
S3-isopropyl-5-methylphenol	**1.55**	**1.76**	**2.06**	**2.57**	**2.87**	**2.36**	**4.38**	**6.11**	**1.96**	**2.69**
Y3-methyl-5-isopropylphenol	0.04	0.07	0.09	0.13	0.15	0.10	0.17	0.29	0.03	0.05
S4-isopropyl-3-methylphenol	**2.45**	**2.90**	**4.54**	**5.93**	**6.19**	**9.46**	**5.20**	**5.77**	**2.69**	**3.21**
Y3-methyl-4-isopropylphenol	0.07	0.11	0.19	0.29	0.33	0.39	0.20	0.28	0.04	0.06
S2-isopropyl-3-methylphenol	**3.91**	**4.19**	**8.78**	**10.75**	**12.28**	**11.81**	**9.06**	**6.75**	**5.40**	**5.45**
Y3-methyl-2-isopropylphenol	0.11	0.16	0.38	0.53	0.66	0.49	0.34	0.32	0.08	0.10
Thymol	79.47	79.35	73.46	72.56	71.08	65.28	70.33	72.36	67.07	68.14
3-methyl-5-isopropylphenol	4.03	4.11	3.55	3.67	3.89	3.46	6.98	9.07	6.41	7.55
3-methyl-2-isopropylphenol	6.37	6.77	7.84	8.45	8.39	13.90	8.28	8.56	8.81	9.00
3-methyl-4-isopropylphenol	10.14	9.77	15.15	15.32	16.64	17.36	14.42	10.02	17.71	15.30
STotal.Isomer	**38.50**	**42.91**	**57.93**	**70.20**	**73.77**	**68.05**	**62.80**	**67.42**	**30.49**	**35.62**
YTotal.Isomer	1.05	1.64	2.48	3.46	3.96	2.81	2.37	3.24	0.44	0.64
Slights	3.80	3.62	2.95	2.27	2.27	2.53	2.99	3.40	5.46	4.55
Ylights	0.10	0.14	0.13	0.11	0.12	0.10	0.11	0.16	0.08	0.08
SC-10	19.75	22.13	9.31	4.67	2.64	1.83	3.33	4.94	2.47	3.63
YC-10	0.54	0.84	0.40	0.23	0.14	0.08	0.13	0.24	0.04	0.06
Sdi-isopropylated	0.54	0.58	0.30	0.56	0.96	0.58	0.42	0.28	-	-
Ydi-isopropylated	0.01	0.02	0.01	0.03	0.05	0.02	0.02	0.01	-	-
Sheavies	6.31	7.71	13.08	10.47	10.24	14.14	11.04	10.36	7.80	14.49
Yheavies	0.17	0.29	0.56	0.52	0.55	0.58	0.42	0.50	0.11	0.26
Sether	1.39	1.19	2.97	3.10	3.70	5.98	6.31	3.67	6.20	3.81

Table 0.44: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-21	MR-22	MR-23	MR-24	MR-25	MR-26	MR-27	MR-28	MR-29	MR-30
Time on Stream	281:34:37	309:39:37	319:52:37	342:40:37	353:19:37	364:28:37	375:51:37	388:30:37	442:02:37	449:27:37
Temperature	325	325	325	325	325	325	325	325	325	325
Entry Temperature	64	74	73	77	77	77	78	77	77	77
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	1.58	1.38	1.42	1.72	1.15	1.04	0.98	1.04	1.00	1.06
Thymol Selectivity	22.30	19.41	15.01	27.88	17.06	12.43	7.41	13.15	10.50	14.04
Thymol Yield	0.35	0.27	0.21	0.48	0.20	0.13	0.07	0.14	0.11	0.15
S3-isopropyl-5-methylphenol	**2.31**	**2.29**	**1.78**	**5.89**	**3.83**	**2.39**	**1.05**	**0.78**	**0.47**	**0.98**
Y3-methyl-5-isopropylphenol	0.04	0.03	0.03	0.10	0.04	0.02	0.01	0.01	0.00	0.01
S4-isopropyl-3-methylphenol	**3.33**	**3.13**	**2.71**	**3.73**	**2.56**	**1.77**	**0.85**	**1.94**	**1.47**	**2.24**
Y3-methyl-4-isopropylphenol	0.05	0.04	0.04	0.06	0.03	0.02	0.01	0.02	0.01	0.02
S2-isopropyl-3-methylphenol	**5.53**	**4.35**	**3.89**	**3.03**	**2.31**	**2.12**	**2.17**	**3.40**	**3.44**	**4.03**
Y3-methyl-2-isopropylphenol	0.09	0.06	0.06	0.05	0.03	0.02	0.02	0.04	0.03	0.04
Thymol	66.64	66.50	64.18	68.78	66.23	66.45	64.53	68.21	66.13	65.97
3-methyl-5-isopropylphenol	6.89	7.86	7.61	14.53	14.88	12.78	9.13	4.07	2.97	4.60
3-methyl-2-isopropylphenol	9.95	10.73	11.58	9.20	9.92	9.45	7.44	10.07	9.25	10.51
3-methyl-4-isopropylphenol	16.52	14.91	16.64	7.48	8.97	11.32	18.90	17.65	21.65	18.92
STotal.Isomer	**33.46**	**29.19**	**23.39**	**40.53**	**25.76**	**18.71**	**11.48**	**19.28**	**15.87**	**21.28**
YTotal.Isomer	0.53	0.40	0.33	0.70	0.30	0.19	0.11	0.20	0.16	0.23
Slights	4.94	5.78	7.21	5.08	6.98	8.01	7.44	7.31	7.73	6.57
Ylights	0.08	0.08	0.10	0.09	0.08	0.08	0.07	0.08	0.08	0.07
SC-10	1.30	0.94	1.33	2.04	2.26	0.89	1.95	0.20	-	-
YC-10	0.02	0.01	0.02	0.04	0.03	0.01	0.02	0.00	-	-
Sdi-isopropylated	-	-	-	-	-	-	-	-	-	-
Ydi-isopropylated	-	-	-	-	-	-	-	-	-	-
Sheavies	12.10	12.53	20.06	14.34	6.63	7.07	7.17	6.72	6.48	7.62
Yheavies	0.19	0.17	0.28	0.25	0.08	0.07	0.07	0.07	0.06	0.08
Sether	6.40	4.69	3.85	0.92	1.21	1.65	2.12	3.02	3.31	2.97

Table 0.45: Conversion, selectivity and yield data for microchannel reactor (cont.)

	MR-31	MR-32	MR-33	MR-34	MR-35	MR-36	MR-37
Time on Stream	451:02:37	457:30:37	463:20:37	475:24:37	480:11:37	489:30:37	499:54:37
Temperature	275	275	274	275	275	274	275
Entry Temperature	76	74	76	76	77	78	78
WHSV	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Pump Rate (ml/min)	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Gauge Pressure (bar)	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3
Conversion	1.00	1.12	1.68	1.89	1.88	1.97	2.11
Thymol Selectivity	9.54	13.03	25.88	29.59	25.26	24.05	24.40
Thymol Yield	0.10	0.15	0.43	0.56	0.47	0.47	0.51
S3-isopropyl-5-methylphenol	**0.59**	**0.88**	**1.36**	**1.44**	**0.93**	**1.78**	**1.02**
Y3-methyl-5-isopropylphenol	0.01	0.01	0.02	0.03	0.02	0.04	0.02
S4-isopropyl-3-methylphenol	**1.49**	**2.19**	**3.56**	**4.10**	**3.55**	**4.17**	**3.93**
Y3-methyl-4-isopropylphenol	0.01	0.02	0.06	0.08	0.07	0.08	0.08
S2-isopropyl-3-methylphenol	**2.94**	**4.47**	**8.50**	**9.68**	**10.05**	**8.85**	**10.40**
Y3-methyl-2-isopropylphenol	0.03	0.05	0.14	0.18	0.19	0.17	0.22
Thymol	65.52	63.34	65.85	66.03	63.49	61.89	61.39
3-methyl-5-isopropylphenol	4.04	4.29	3.45	3.22	2.33	4.59	2.56
3-methyl-2-isopropylphenol	10.24	10.62	9.07	9.15	8.93	10.74	9.89
3-methyl-4-isopropylphenol	20.19	21.74	21.64	21.60	25.25	22.78	26.16
STotal.Isomer	**14.55**	**20.58**	**39.31**	**44.82**	**39.79**	**38.86**	**39.74**
YTotal.Isomer	0.15	0.23	0.66	0.85	0.75	0.77	0.84
Slights	7.00	6.79	4.68	4.40	3.50	4.06	4.17
Ylights	0.07	0.08	0.08	0.08	0.07	0.08	0.09
SC-10	-	-	0.43	0.35	0.32	0.73	-
YC-10	-	-	0.01	0.01	0.01	0.01	-
Sdi-isopropylated	-	-	-	0.36	0.49	0.20	0.36
Ydi-isopropylated	-	-	-	0.01	0.01	0.00	0.01
Sheavies	8.75	7.31	10.50	8.76	7.94	11.51	11.53
Yheavies	0.09	0.08	0.18	0.17	0.15	0.23	0.24
Sether	3.29	4.87	7.76	9.83	15.82	14.14	16.12

Table 0.46: GC raw data for H-MFI-90 powder repeat

		PW-1	PW-3	PW-5	PW-7	PW-11	PW-15	PW-20	PW-23	PW-28	PW-29
Time on Stream		07:52:00	08:58:06	11:00:07	13:04:06	20:02:06	31:58:07	38:00:07	41:00:06	46:56:06	55:00:00
Entry Temperature		90	91	91	93	92	92	92	92	91	92
Temperature		275	275	275	274	275	274	275	274	275	275
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	6.8	5.2	5.4	7.2	14.6	15.4	33.9	21.9	36.8	24.6
???	± 5.04	30.1	2.5	1.5	1.4	1.2	1.1	1.3			
phenol	± 5.26	1.9			1.9	2.5	2.6	6.5	4.3	6.9	4.2
o-Cresol	± 5.35	275.3	18.3	13.1	6.3	6.6	6.6	13.6	7.4	10.3	5.2
p-Cresol	± 5.60	732.4	93.7	67.8	59.3	65.4	65.3	136.6	80.2	103	55.1
m-Cresol	± 5.80	14755.3	8777.3	6587.4	6225.9	7312.7	7707.4	17162.3	10134.3	13195.9	6997.1
???	± 6.00	7.2	5.9	4.4	4.3	5.6	5.9	12	7.1	9	4.9
2,4-Xylenol	± 6.20	28.1	5.9	3	2	2.5	2.1	3.9	2	2.9	1.6
2,5-Xylenol	± 6.50	6.5	6.4	4.7	3.7	4.8	4.6	9.1	4.4	7.4	3.6
2,3-Xylenol	± 6.74	4.3	6.8	4.5	4.7	3.8	4.9	6.4	3.1	5.6	3
???	± 6.90	23.8	13.8		6.8	6.4	5.6	9.1	4.5	6.1	4.4
???	± 7.03	52.9									
???	± 7.16	49.3	9.7	15.8	4.3	4	3.2	4.8	2.5	2.9	1.9
2-Isopropyl-4-methyl Phenol	± 7.30	51.5	25	20.2	17.7	17.1	15.6	25.3	14.7	20.3	11.5
???	± 7.49	13.8	7.3	1.7	2	1.1	1.3	1.5	2.3	1.8	2
Thymol isomer (2,3)	± 7.60	50.7	236	202.7	201.3	223.4	230.4	426	246	371.1	202.8
???	± 7.73	189.1	46.1	33.4	27.5	23.1	21.2	32.9	18.9	22.8	10.5
Thymol	± 7.90	1881.5	4413.6	3579.6	3302.2	3259.2	3104.5	5243.5	2926.2	3927.4	2123.2
????	± 8.19	244.3	51.3	37.5	32	27.2	25.1	38.3	22.3	28.4	15.7
????	± 8.33	971.4	567.3	415	348.9	307.3	280.2	436.5	242.4	287.3	158.1
6-n-Propyl-3-Methyl Phenol	± 8.40	10.6	42.8	38.6	35.8	33.3	30.4	57	26	42	24.7
2,6-Diisoprop.-3-Met. Phen.	± 8.55	418.4	84.4	59.4	47.1	37.5	34.4	50.5	28.3	34.4	18.8
5,3 Thymol isomer	± 8.67	541	294.4	226.8	198.8	175.9	160.8	244.9	136.4	183.4	95.2
4,3 Thymol isomer	± 8.78	495.8	1124.5	934.4	866.8	864.9	839	1343.7	745.6	1071	565.6
C-13 fraction (13.02)	± 8.83	34.6									
????	± 9.22	156.8	63.8	41.2	31.6	19.8	15.4	16.5	9.3	10.9	6
????	± 9.48	141.4	38.3	28.7	24.6	22.3	20.9	31.1	18.6	23.9	11.6
????	± 9.60	13.8	2.1								
????	± 10.30	133.2	75.1	44.2	29.6	16.7	10.7	11.4	5.6	7	4
????	± 10.70	85.4	5.3	2.8							
4,6-Diisoprop.-3-Met. Phen.	± 11.18	102.4	174.8	139.1	119.9	96.1	83	103.8	57.9	89.8	52.6
????	± 11.30	33									
????	± 11.80	15.9	4.8								
????	± 12.09	60.4									
????	± 12.21	8.1	11.2	7.8	7.8	6.4	5.2	6.5	4.4	6.2	4.2
5,6-Diisoprop.-3-Met. Phen.	± 12.70	39.3	32	27.5	24.1	21	20.2	25.9	13.4	23	12.9
Heavies	± 13.04	21	25.4	11.8	10.4	3.1					
Heavies		89.5	12.5	13.5	11.8	10.6	15.6	24	15	16.5	8.6

Table 0.47: GC raw data for H-MFI-90 powder repeat (cont.)

		PW-35	PW-37	PW-39	PW-43	PW-46	PW-47	PW-48	PW-49	PW-50	PW-51
Time on Stream		60:00:07	68:00:07	81:00:06	89:00:06	93:50:06	103:44:21	104:00:21	105:00:21	106:00:21	107:00:21
Entry Temperature		93	86	93	94	94	92	92	92	92	93
Temperature		274	275	276	275	275	275	274	275	275	274
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (ml/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	42	32.6	38.5	39.9	48.5	29.8	40.1	46.7	42.8	38.2
???	± 5.04										
phenol	± 5.26	8.5	6.1	8.2	7.6	9.3	5.7	7.1	8.6	7.2	6.5
o-Cresol	± 5.35	9.7	6.7	7.9	8.1	10.8	5.2	5.9	7.3	5.8	5.5
p-Cresol	± 5.60	98.3	71.2	87.9	85.6	105.6	56.4	60	78.4	61.7	53.8
m-Cresol	± 5.80	13158.4	9503.9	11963.4	11910.2	14707.3	7790.2	8466.1	10946.7	8663.9	7622
???	± 6.00	8.9	5.5	7	8.3	8.3	5.4	5.8	7.5	5.6	5
2,4-Xylenol	± 6.20	8.8	2	2.6	2	2	1.3	1	1.8	1.3	3.3
2,5-Xylenol	± 6.50	1	5.1	5.2	4.6	5.8	3.2	2.9	5	3.5	
2,3-Xylenol	± 6.74	4.6	2.8	3.8	2.4	3.1	1.5	1.7	2.7	2.3	2.1
???	± 6.90	5.1	3	2.7	3.1	3.6	1.4	1.1	2	1.8	1.6
???	± 7.03										
???	± 7.16	2.3	2.2	1.8	1.6	1.8	0.9	1.5	1.2	1.1	1.3
2-Isopropyl-4-methyl Phenol	± 7.30	16.3	10.1	11.7	10.5	11.2	6.2	6.8	8.7	6.5	5.7
???	± 7.49	0.7	1.4	1.9							
Thymol isomer (2,3)	± 7.60	335	235.2	260.7	241.7	287.1	154.6	179.3	234.8	183.5	152.6
???	± 7.73	16.7	12	13	12.2	13.6	7	7	8.9	5.6	5.8
Thymol	± 7.90	3096.2	2125	2300.1	2072.6	2471.2	1222.1	1337.1	1767.3	1348.5	1098
????	± 8.19	21.5	15	16.1		14.6	7.9	8.3	12	8.1	7
????	± 8.33	213.6	146.9	165.1	144.6	170.8	84.7	84.5	110.7	84	67.4
6-n-Propyl-3-Methyl Phenol	± 8.40	30.9	21.3	21.1	19.8	20.7	10.2	14.5	18.4	14.4	11
2,6-Diisoprop.-3-Met. Phen.	± 8.55	25.6	17.3	19.3	17.1	19	8.9	10.1	13.3	10	7.4
5,3 Thymol isomer	± 8.67	138.4	93.5	98.6	86.4	101.4	49.1	56.7	76.9	55.9	46.1
4,3 Thymol isomer	± 8.78	839.3	559.6	603.8	525.3	611.4	295.3	349.4	479.2	354.5	287
C-13 fraction (13.02)	± 8.83										
????	± 9.22	5.4	5	3.9	2.8	4.2	2	2.2	1.8	1	1.6
????	± 9.48	17.5	13	12.3	11.5	12.7	6.3	6.7	9.4	7	5.4
????	± 9.60										
????	± 10.30	3.6	2.4	1.5							
????	± 10.70										
4,6-Diisoprop.-3-Met. Phen.	± 11.18	64.7	44.6	41.2	34.1	39	18.2	24.7	33.9	23.9	19.5
????	± 11.30										
????	± 11.80										
????	± 12.09										
????	± 12.21	4.1	3.2	2.4	3.5	3.1	1.4	1.5	1.6	1.8	1.1
5,6-Diisoprop.-3-Met. Phen.	± 12.70	16.8	11.6	10	7.7	6.7	5.3	5.8	8.2	8.3	6.6
Heavies	± 13.04										
Heavies		12.7	13.2	12.5	28.4	14.8	10.9	14.1	15.4	12.5	11.2

Table 0.48: GC raw data for H-MFI-90 powder repeat (cont.)

		PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59	PW-60	PW-61	PW-62	PW-63	PW-64	PW-65	PW-66
Time on Stream		132:00	133:00	134:00	135:00	135:54	152:00	163:14	179:00	181:00	182:48	188:00	188:56	190:00	191:00	198:04
Entry Temperature		92	91	92	93	94	94	96	95	95	95	89	89	90	89	90
Temperature		276	275	275	275	275	275	274	275	274	274	275	276	276	275	276
WHSV		0.72	0.72	0.72	0.72	0.72	0.3	0.3	0.3	0.3	0.3	1. 2	1. 2	1. 2	1. 2	1. 2
Pump Rate (ml/min)		0.12	0.12	0.12	0.12	0.12	0.05	0.05	0.05	0.05	0.05	0.2	0.2	0.2	0.2	0.2
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	75.7	41.3	54.2	41.8	58.6	30.4	34	43	47	32.8	56.9	68.3	60.8	84.2	65
???	± 5.04							2.9								
phenol	± 5.26	14.4	8.4	9.9	8.4	10.8	6.1	11.3	8.7	8.7	6.4	8.1	10.1	7.2	9.7	9.4
o-Cresol	± 5.35	9.4	6.2	8.1	6	9.2	4.1	7.2	9.2	9.9	5.8	6.1	9.3	8	11.4	13.1
p-Cresol	± 5.60	130.9	66.8	86.4	63.2	95	68.9	84.4	91.6	101.6	73.8	74.6	99.5	88.6	127.9	130.5
m-Cresol	± 5.80	18759	9558.4	12262.7	9007	13685.5	8584.8	10109	11629	12918.7	9199.8	11222.9	15186.5	13580.7	19400.6	20133.4
???	± 6.00	20.7	11.5	7.1	6.2	8.1	4.8	24.5	8.5	16	6.7	6.3		7	36.8	11.7
2,4-Xylenol	± 6.20	3.1	1.8	1.3	1.2	5.3	1.6	13.2	4	3.6	4.8	1.1	1.8	1.9	1.2	2.1
2,5-Xylenol	± 6.50	8.5	3.6	4.5	3.7		5.5	10	6.9	6		3.9	5.7	4.6	2.5	7
2,3-Xylenol	± 6.74	4.5	2.1	2.8	1.9	2.8	3.9	3.8	4.8	5.2	3.9	1.6	2	1.2	7.7	1.2
???	± 6.90	3	3.2	2.8	2.7	2.5	5.2	4.9	6.3	4.8	3.8					
???	± 7.03															
???	± 7.16	2	1.4	1.2	1.6	1.3	2.4	3.7	3.8	4	3.5					
2-Isopropyl-4-methyl Phenol	± 7.30	15.7	7.4	9.4	7	9.1	17	17.9	21.7	24.2	17.1	3.9	5.1	4	4.5	4
???	± 7.49						1.8	2.3	1.6	2.1	1.6					
Thymol isomer (2,3)	± 7.60	388.2	199.5	256.9	188.6	255.6	323.6	387.4	428.7	476.7	340	132	164.7	134.5	172.9	139.3
???	± 7.73	14.2	5.7	9.5	6.5	7.3	17.2	21	22.2	23.7	22.7	3.6	4.7	3.6	15.2	3.7
Thymol	± 7.90	2861.9	1449.7	1862.6	1341.9	1813.6	3071	3648	3965.4	4337.3	3130.7	746.9	956.6	766.8	999.6	775.2
????	± 8.19	18.7	9.4	12.5	8.3	8.6	21	24	26.4	28.3	20.8	4.4	5.6	4.8	6.5	4.1
????	± 8.33	170.9	89	110.8	80.1	106.2	203.3	239.5	254.4	276.3	201.3	38.4	50.7	41	53.3	40.6
6-n-Propyl-3-Methyl Phenol	± 8.40	30.3	15.3	19.1	15	19.3	53.7	112.5	70.9	74.8	56.6	6.3	6.1	4.7	25	3.6
2,6-Diisoprop.-3-Met. Phen.	± 8.55	20.4	10.9	13.2	9.8	12.7	24	35	28.9	31.6	24.3	5	6.8	5.3	9.5	5.2
5,3 Thymol isomer	± 8.67	126.8	63.8	76.5	57.9	74.8	141.6	161.7	165.8	192.1	141.5	32.2	42.4	33.6	43.6	33.9
4,3 Thymol isomer	± 8.78	778.1	392.7	473.5	361.8	478.9	693.4	859.9	909.8	996.2	739.6	216.2	294.8	223.3	289.5	214.4
C-13 fraction (13.02)	± 8.83															
????	± 9.22	4.4	2.8	2.4	2.1	3.1	9.7	20.2	11.8	11.6	7.9					
????	± 9.48	18.8	8.6	9.5	7.2	11.1	17.9	22.4	24.5	26.9	19.6	3.5	4.7	4.9	5.3	4.3
????	± 9.60															
????	± 10.30						4	7.9	7.4	5.9	6.8					
????	± 10.70							12.3								
4,6-Diisoprop.-3-Met. Phen.	± 11.18	54.8	29.9	33.9	27.4	32.6	98.9	133.6	128.6	139	101.4	9.3	11.3	8	7.7	5.8
????	± 11.30															
????	± 11.80															
????	± 12.09															
????	± 12.21	4.8	4.3	7.7	5.3	4.2	3.4	5.3	4.8	3.9	4.1					
5,6-Diisoprop.-3-Met. Phen.	± 12.70	14.4	8.1	8.2	6.3	8.3	21.3	24.3	26.3	28.5	23.1	4.2	3.8	4.4	3.4	1.9
Heavies	± 13.04															
Heavies		14.2	14.4	15.2	14.5	14.3	11.2	9	18.5	18.1	16.9	12.6	12.5	13.2	12.4	12.2

Table 0.49: GC raw data for H-MFI-90 powder repeat (cont.)

		PW-67	PW-68	PW-69	PW-70	PW-71	PW-72	PW-73	PW-74	PW-75	PW-76	PW-77	PW-78
Time on Stream		201:00:55	201:30:55	201:58:55	205:00:55	205:30:55	206:00:55	206:30:55	232:10:55	233:30:55	236:32:55	238:30:55	246:36:55
Entry Temperature		90	90	89	85	85	85	85	93	93	92	92	90
Temperature		274	275	275	275	275	275	275	274	275	275	275	275
WHSV		1.81	1.81	1.81	3.62	3.62	3.62	3.62	0.96	0.96	0.96	0.96	0.96
Pump Rate (ml/min)		0.302	0.302	0.302	0.604	0.604	0.604	0.604	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	91	99.5	110.3	9.6	14.5	13.6	12.9	61.2	33	53.4	45.5	67.1
???	± 5.04												
phenol	± 5.26	2.4	2.6	2.9									
o-Cresol	± 5.35	10.3	10.8	13.1	8.3	10.1	8.4	7.9	10.2	3.2	8	8.3	14
p-Cresol	± 5.60	105.9	115.1	131.9	93	89	96	84.7	107.6	47.8	81.7	73.9	136.3
m-Cresol	± 5.80	16737.3	18133.1	20848.9	9370.5	17450.9	15342.4	13510.9	17131.1	7528.3	13072.5	11793	21803.7
???	± 6.00	9.6	10.6	11.7	5.3	10.4	8.2	8.1	10.5	4.2	7.9	6.7	12.5
2,4-Xylenol	± 6.20	1.5	1.7	1.8	1	2	1.9	1.4	1.1	1	1.2	1.1	1.4
2,5-Xylenol	± 6.50	5.3	6.4	6.7	3.2	6.1	5.5	4.7	5.2	2.5	4.5	4.2	7.1
2,3-Xylenol	± 6.74												
???	± 6.90												
???	± 7.03												
???	± 7.16												
2-Isopropyl-4-methyl Phenol	± 7.30	0.7	1.2	1.8									
???	± 7.49												
Thymol isomer (2,3)	± 7.60	46.3	44	50.9	2.6	4.6	4.4	3.4	22.3	9.7	17.1	13.5	24.9
???	± 7.73												
Thymol	± 7.90	222.2	216.5	243.1	5.9	9.4	8.2	6.5	37.6	15.6	28.6	23.1	41.6
????	± 8.19	1.3	1.3	1.2									
????	± 8.33	9.4	9	10.2									
6-n-Propyl-3-Methyl Phenol	± 8.40												
2,6-Diisoprop.-3-Met. Phen.	± 8.55												
5,3 Thymol isomer	± 8.67	10.7	10.4	11.3	0.6	0.9	0.6	1	2.9	1.4	1.1	1.7	2.9
4,3 Thymol isomer	± 8.78	64.5	64	71.9	1.9	3.3	2.7	2.8	10.9	4.6	7.3	6.1	12.7
C-13 fraction (13.02)	± 8.83												
????	± 9.22												
????	± 9.48												
????	± 9.60												
????	± 10.30												
????	± 10.70												
4,6-Diisoprop.-3-Met. Phen.	± 11.18	2.2	2.3	2					1.3	0.6	1.1	1	1.9
????	± 11.30												
????	± 11.80												
????	± 12.09												
????	± 12.21												
5,6-Diisoprop.-3-Met. Phen.	± 12.70												
Heavies	± 13.04												
Heavies		9.9	11.9	10.4	11.3	11.7	11.1	11.4	8.8	9.5	9.8	9.6	8.9

Table 0.50: Product composition (%) for H-MFI-90 powder repeat

		PW-1	PW-3	PW-5	PW-7	PW-11	PW-15	PW-20	PW-23	PW-28	PW-29
Time on Stream		07:52:00	08:58:06	11:00:07	13:04:06	20:02:06	31:58:07	38:00:07	41:00:06	46:56:06	55:00:00
Entry Temperature		90	91	91	93	92	92	92	92	91	92
Temperature		275	275	275	274	275	274	275	274	275	275
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.04	0.03	0.04	0.05	0.10	0.10	0.11	0.12	0.15	0.19
???	± 5.04	0.15	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
phenol	± 5.26	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.03	0.03
o-Cresol	± 5.35	1.40	0.13	0.12	0.06	0.06	0.06	0.06	0.06	0.06	0.06
p-Cresol	± 5.60	3.72	0.68	0.64	0.60	0.60	0.59	0.60	0.60	0.59	0.59
m-Cresol	± 5.80	74.94	63.29	61.83	62.72	66.93	69.12	74.93	75.94	75.14	74.78
???	± 6.00	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.11	0.03	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01
2,5-Xylenol	± 6.50	0.03	0.04	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
2,3-Xylenol	± 6.74	0.02	0.04	0.03	0.04	0.03	0.03	0.02	0.02	0.02	0.02
???	± 6.90	0.09	0.08	-	0.05	0.04	0.04	0.03	0.03	0.03	0.04
???	± 7.03	0.21	-	-	-	-	-	-	-	-	-
???	± 7.16	0.19	0.05	0.11	0.03	0.03	0.02	0.02	0.01	0.01	0.02
2-Isopropyl-4-methyl Phenol	± 7.30	0.20	0.14	0.15	0.14	0.12	0.11	0.08	0.08	0.09	0.09
???	± 7.49	0.05	0.03	0.01	0.02	0.01	0.01	0.01	0.01	0.01	0.02
Thymol isomer (2,3)	± 7.60	0.18	1.17	1.30	1.39	1.40	1.42	1.28	1.26	1.45	1.49
???	± 7.73	0.66	0.23	0.22	0.19	0.15	0.13	0.10	0.10	0.09	0.08
Thymol	± 7.90	6.55	21.83	23.04	22.82	20.46	19.10	15.70	15.04	15.34	15.56
????	± 8.19	0.85	0.25	0.24	0.22	0.17	0.15	0.11	0.11	0.11	0.12
????	± 8.33	3.38	2.81	2.67	2.41	1.93	1.72	1.31	1.25	1.12	1.16
6-n-Propyl-3-Methyl Phenol	± 8.40	0.04	0.21	0.25	0.25	0.21	0.19	0.17	0.13	0.16	0.18
2,6-Diisoprop.-3-Met. Phen.	± 8.55	1.11	0.32	0.29	0.25	0.18	0.16	0.12	0.11	0.10	0.10
5,3 Thymol isomer	± 8.67	1.88	1.46	1.46	1.37	1.10	0.99	0.73	0.70	0.72	0.70
4,3 Thymol isomer	± 8.78	1.73	5.56	6.01	5.99	5.43	5.16	4.02	3.83	4.18	4.15
C-13 fraction (13.02)	± 8.83	0.09	-	-	-	-	-	-	-	-	-
????	± 9.22	0.42	0.24	0.20	0.17	0.09	0.07	0.04	0.04	0.03	0.03
????	± 9.48	0.37	0.14	0.14	0.13	0.11	0.10	0.07	0.07	0.07	0.06
????	± 9.60	0.04	0.01	-	-	-	-	-	-	-	-
????	± 10.30	0.35	0.28	0.22	0.16	0.08	0.05	0.03	0.02	0.02	0.02
????	± 10.70	0.23	0.02	0.01	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.27	0.66	0.68	0.63	0.46	0.39	0.24	0.23	0.27	0.29
????	± 11.30	0.09	-	-	-	-	-	-	-	-	-
????	± 11.80	0.04	0.02	-	-	-	-	-	-	-	-
????	± 12.09	0.16	-	-	-	-	-	-	-	-	-
????	± 12.21	0.02	0.04	0.04	0.04	0.03	0.02	0.01	0.02	0.02	0.02
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.10	0.12	0.13	0.13	0.10	0.09	0.06	0.05	0.07	0.07
Heavies	± 13.04	0.06	0.10	0.06	0.05	0.01	-	-	-	-	-
Heavies		0.24	0.16	0.08	0.06	0.05	0.07	0.05	0.06	0.05	0.05

Table 0.51: Product composition (%) for H-MFI-90 powder repeat (cont.)

		PW-35	PW-37	PW-39	PW-43	PW-46	PW-47	PW-48	PW-49	PW-50	PW-51
Time on Stream		60:00:07	68:00:07	81:00:06	89:00:06	93:50:06	103:44:21	104:00:21	105:00:21	106:00:21	107:00:21
Entry Temperature		93	86	93	94	94	92	92	92	92	93
Temperature		274	275	276	275	275	275	274	275	275	274
WHSV		0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)		0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.18	0.20	0.19	0.20	0.20	0.23	0.29	0.26	0.30	0.31
???	± 5.04	-	-	-	-	-	-	-	-	-	-
phenol	± 5.26	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.05	0.05	0.05
o-Cresol	± 5.35	0.06	0.06	0.05	0.06	0.06	0.06	0.06	0.06	0.06	0.06
p-Cresol	± 5.60	0.59	0.60	0.60	0.60	0.60	0.61	0.60	0.60	0.60	0.60
m-Cresol	± 5.80	79.10	79.92	82.16	83.60	84.17	84.90	84.55	84.23	84.72	85.60
???	± 6.00	0.04	0.04	0.04	0.04	0.04	0.05	0.04	0.04	0.04	0.04
2,4-Xylenol	± 6.20	0.04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.03
2,5-Xylenol	± 6.50	0.00	0.03	0.03	0.02	0.03	0.03	0.02	0.03	0.03	-
2,3-Xylenol	± 6.74	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.02	0.02	0.02
???	± 6.90	0.02	0.02	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
???	± 7.03	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
2-Isopropyl-4-methyl Phenol	± 7.30	0.08	0.07	0.06	0.06	0.05	0.05	0.05	0.05	0.05	0.05
???	± 7.49	0.00	0.01	0.01	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	1.38	1.36	1.23	1.16	1.13	1.16	1.23	1.24	1.23	1.18
???	± 7.73	0.07	0.07	0.06	0.06	0.05	0.05	0.05	0.05	0.04	0.04
Thymol	± 7.90	12.77	12.26	10.83	9.98	9.70	9.13	9.16	9.33	9.04	8.46
????	± 8.19	0.09	0.09	0.08	0.06	0.06	0.06	0.06	0.06	0.05	0.05
????	± 8.33	0.88	0.85	0.78	0.70	0.67	0.63	0.58	0.58	0.56	0.52
6-n-Propyl-3-Methyl Phenol	± 8.40	0.13	0.12	0.10	0.10	0.08	0.08	0.10	0.10	0.10	0.08
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.08	0.08	0.07	0.06	0.06	0.05	0.05	0.05	0.05	0.04
5,3 Thymol isomer	± 8.67	0.57	0.54	0.46	0.42	0.40	0.37	0.39	0.41	0.37	0.36
4,3 Thymol isomer	± 8.78	3.46	3.23	2.84	2.53	2.40	2.21	2.39	2.53	2.38	2.21
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-
????	± 9.22	0.02	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
????	± 9.48	0.05	0.06	0.04	0.04	0.04	0.04	0.03	0.04	0.04	0.03
????	± 9.60	-	-	-	-	-	-	-	-	-	-
????	± 10.30	0.01	0.01	0.01	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.20	0.20	0.15	0.12	0.12	0.10	0.13	0.14	0.12	0.11
????	± 11.30	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.05	0.05	0.04	0.03	0.04	0.03	0.03	0.03	0.04	0.04
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-
Heavies		0.04	0.06	0.04	0.10	0.04	0.06	0.07	0.06	0.06	0.07

Table 0.52: Product composition (%) for H-MFI-90 powder repeat (cont.)

		PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59	PW-60	PW-61	PW-62	PW-63	PW-64	PW-65	PW-66
Time on Stream		132:00	133:00	134:00	135:00	135:54	152:00	163:14	179:00	181:00	182:48	188:00	188:56	190:00	191:00	198:04
Entry Temperature		92	91	92	93	94	94	96	95	95	95	89	89	90	89	90
Temperature		276	275	275	275	275	275	274	275	274	274	275	276	276	275	276
WHSV		0.72	0.72	0.72	0.72	0.72	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (m/min)		0.12	0.12	0.12	0.12	0.12	0.05	0.05	0.05	0.05	0.05	0.2	0.2	0.2	0.2	0.2
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.25	0.26	0.27	0.28	0.27	0.18	0.17	0.19	0.19	0.19	0.34	0.30	0.30	0.29	0.22
???	± 5.04	-	-	-	-	-	-	0.02	-	-	-	-	-	-	-	-
phenol	± 5.26	0.05	0.05	0.05	0.06	0.05	0.04	0.06	0.04	0.04	0.04	0.05	0.04	0.04	0.03	0.03
o-Cresol	± 5.35	0.04	0.06	0.06	0.06	0.06	0.03	0.05	0.06	0.06	0.05	0.05	0.06	0.05	0.05	0.06
p-Cresol	± 5.60	0.59	0.59	0.60	0.60	0.60	0.58	0.60	0.57	0.58	0.58	0.61	0.61	0.61	0.62	0.62
m-Cresol	± 5.80	84.93	84.90	85.11	85.12	86.60	72.03	71.29	72.91	73.18	72.80	92.06	92.43	93.08	93.41	94.97
???	± 6.00	0.07	0.08	0.04	0.04	0.04	0.03	0.13	0.04	0.07	0.04	0.04	-	0.04	0.14	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.03	0.01	0.07	0.02	0.02	0.03	0.01	0.01	0.01	0.00	0.01
2,5-Xylenol	± 6.50	0.03	0.02	0.02	0.03	-	0.04	0.05	0.03	0.03	-	0.02	0.03	0.02	0.01	0.03
2,3-Xylenol	± 6.74	0.02	0.01	0.01	0.01	0.01	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.03	0.00
???	± 6.90	0.01	0.02	0.01	0.02	0.01	0.03	0.03	0.03	0.02	0.02	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	-	-	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	0.05	0.05	0.05	0.05	0.04	0.11	0.10	0.10	0.11	0.10	0.02	0.02	0.02	0.02	0.01
???	± 7.49	-	-	-	-	-	0.01	0.01	0.01	0.01	0.01	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	1.21	1.22	1.22	1.22	1.11	1.86	1.87	1.84	1.85	1.85	0.74	0.69	0.63	0.57	0.45
???	± 7.73	0.04	0.03	0.05	0.04	0.03	0.10	0.10	0.10	0.09	0.12	0.02	0.02	0.02	0.05	0.01
Thymol	± 7.90	8.89	8.83	8.87	8.70	7.87	17.67	17.65	17.05	16.85	16.99	4.20	3.99	3.60	3.30	2.51
????	± 8.19	0.06	0.06	0.06	0.05	0.04	0.12	0.12	0.11	0.11	0.11	0.02	0.02	0.02	0.02	0.01
????	± 8.33	0.53	0.54	0.53	0.52	0.46	1.17	1.16	1.09	1.07	1.09	0.22	0.21	0.19	0.18	0.13
6-n-Propyl-3-Methyl Phenol	± 8.40	0.09	0.09	0.09	0.10	0.08	0.31	0.54	0.30	0.29	0.31	0.04	0.03	0.02	0.08	0.01
2,6-Diisoprop.-3-Met. Phen.	± 8.55	0.05	0.05	0.05	0.05	0.04	0.11	0.13	0.09	0.09	0.10	0.02	0.02	0.02	0.02	0.01
5,3 Thymol isomer	± 8.67	0.39	0.39	0.36	0.38	0.32	0.81	0.78	0.71	0.75	0.77	0.18	0.18	0.16	0.14	0.11
4,3 Thymol isomer	± 8.78	2.42	2.39	2.25	2.35	2.08	3.99	4.16	3.91	3.87	4.01	1.22	1.23	1.05	0.96	0.69
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.22	0.01	0.01	0.01	0.01	0.01	0.04	0.07	0.04	0.03	0.03	-	-	-	-	-
????	± 9.48	0.04	0.04	0.03	0.04	0.04	0.08	0.08	0.08	0.08	0.08	0.01	0.01	0.02	0.01	0.01
????	± 9.60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 10.30	-	-	-	-	-	0.02	0.03	0.02	0.02	0.03	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	0.05	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.13	0.14	0.12	0.14	0.11	0.43	0.49	0.42	0.41	0.42	0.04	0.04	0.03	0.02	0.01
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	0.01	0.02	0.03	0.03	0.01	0.01	0.02	0.02	0.01	0.02	-	-	-	-	-
5,6-Diisoprop.-3-Met. Phen.	± 12.70	0.03	0.04	0.03	0.03	0.03	0.09	0.09	0.09	0.08	0.10	0.02	0.01	0.02	0.01	0.00
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Heavies		0.03	0.07	0.06	0.07	0.05	0.05	0.03	0.06	0.05	0.07	0.05	0.04	0.05	0.03	0.03

Table 0.53: Product composition (%) for H-MFI-90 powder repeat(cont.)

		PW-67	PW-68	PW-69	PW-70	PW-71	PW-72	PW-73	PW-74	PW-75	PW-76	PW-77	PW-78
Time on Stream		201:00:55	201:30:55	201:58:55	205:00:55	205:30:55	206:00:55	206:30:55	232:10:55	233:30:55	236:32:55	238:30:55	246:36:55
Entry Temperature		90	90	89	85	85	85	85	93	93	92	92	90
Temperature		274	275	275	275	275	275	275	274	275	275	275	275
WHSV		1.81	1.81	1.81	3.62	3.62	3.62	3.62	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)		0.302	0.302	0.302	0.604	0.604	0.604	0.604	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)		2	2	2	2	2	2	2	2	2	2	2	2
ether	± 4.70	0.38	0.39	0.37	0.07	0.06	0.06	0.07	0.25	0.31	0.29	0.27	0.22
???	± 5.04	-	-	-	-	-	-	-	-	-	-	-	-
phenol	± 5.26	0.01	0.01	0.01	-	-	-	-	-	-	-	-	-
o-Cresol	± 5.35	0.06	0.06	0.06	0.09	0.06	0.05	0.06	0.06	0.04	0.06	0.07	0.06
p-Cresol	± 5.60	0.62	0.62	0.62	0.98	0.51	0.62	0.62	0.62	0.63	0.62	0.62	0.62
m-Cresol	± 5.80	97.40	97.53	97.58	98.64	99.19	99.08	99.06	98.67	98.59	98.63	98.66	98.75
???	± 6.00	0.04	0.04	0.04	0.04	0.05	0.04	0.05	0.05	0.04	0.05	0.04	0.04
2,4-Xylenol	± 6.20	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.00
2,5-Xylenol	± 6.50	0.02	0.03	0.02	0.03	0.03	0.03	0.03	0.02	0.03	0.03	0.03	0.02
2,3-Xylenol	± 6.74	-	-	-	-	-	-	-	-	-	-	-	-
???	± 6.90	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.03	-	-	-	-	-	-	-	-	-	-	-	-
???	± 7.16	-	-	-	-	-	-	-	-	-	-	-	-
2-Isopropyl-4-methyl Phenol	± 7.30	0.00	0.00	0.01	-	-	-	-	-	-	-	-	-
???	± 7.49	-	-	-	-	-	-	-	-	-	-	-	-
Thymol isomer (2,3)	± 7.60	0.18	0.16	0.16	0.02	0.02	0.02	0.02	0.09	0.09	0.09	0.08	0.08
???	± 7.73	-	-	-	-	-	-	-	-	-	-	-	-
Thymol	± 7.90	0.89	0.80	0.78	0.04	0.04	0.04	0.03	0.15	0.14	0.15	0.13	0.13
????	± 8.19	0.01	0.00	0.00	-	-	-	-	-	-	-	-	-
????	± 8.33	0.04	0.03	0.03	-	-	-	-	-	-	-	-	-
6-n-Propyl-3-Methyl Phenol	± 8.40	-	-	-	-	-	-	-	-	-	-	-	-
2,6-Diisoprop.-3-Met. Phen.	± 8.55	-	-	-	-	-	-	-	-	-	-	-	-
5,3 Thymol isomer	± 8.67	0.04	0.04	0.04	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
4,3 Thymol isomer	± 8.78	0.26	0.24	0.23	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04
C-13 fraction (13.02)	± 8.83	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.22	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.48	-	-	-	-	-	-	-	-	-	-	-	-
????	± 9.60	-	-	-	-	-	-	-	-	-	-	-	-
????	± 10.30	-	-	-	-	-	-	-	-	-	-	-	-
????	± 10.70	-	-	-	-	-	-	-	-	-	-	-	-
4,6-Diisoprop.-3-Met. Phen.	± 11.18	0.01	0.01	0.00	-	-	-	-	0.00	0.00	0.00	0.00	0.00
????	± 11.30	-	-	-	-	-	-	-	-	-	-	-	-
????	± 11.80	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.09	-	-	-	-	-	-	-	-	-	-	-	-
????	± 12.21	-	-	-	-	-	-	-	-	-	-	-	-
5,6-Diisoprop.-3-Met. Phen.	± 12.70	-	-	-	-	-	-	-	-	-	-	-	-
Heavies	± 13.04	-	-	-	-	-	-	-	-	-	-	-	-
Heavies		0.03	0.03	0.03	0.06	0.03	0.04	0.04	0.03	0.06	0.04	0.04	0.02

Table 0.54: Conversion, selectivity and yield data for H-MFI-90 powder repeat

	PW-1	PW-3	PW-5	PW-7	PW-11	PW-15	PW-20	PW-23	PW-28	PW-29
Time on Stream	07:52:00	08:58:06	11:00:07	13:04:06	20:02:06	31:58:07	38:00:07	41:00:06	46:56:06	55:00:00
Entry Temperature	90	91	91	93	92	92	92	92	91	92
Temperature	275	275	275	274	275	274	275	274	275	275
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	25.06	36.71	38.17	37.28	33.07	30.88	25.07	24.06	24.86	25.22
Thymol Selectivity	26.15	59.45	60.36	61.20	61.88	61.84	62.63	62.52	61.69	61.70
Thymol Yield	6.55	21.83	23.04	22.82	20.46	19.10	15.70	15.04	15.34	15.56
S3-isopropyl-5-methylphenol	**7.52**	**3.97**	**3.82**	**3.68**	**3.34**	**3.20**	**2.93**	**2.91**	**2.88**	**2.77**
Y3-methyl-5-isopropylphenol	1.88	1.46	1.46	1.37	1.10	0.99	0.73	0.70	0.72	0.70
S4-isopropyl-3-methylphenol	**6.89**	**15.15**	**15.76**	**16.06**	**16.42**	**16.71**	**16.05**	**15.93**	**16.82**	**16.44**
Y3-methyl-4-isopropylphenol	1.73	5.56	6.01	5.99	5.43	5.16	4.02	3.83	4.18	4.15
S2-isopropyl-3-methylphenol	**0.70**	**3.18**	**3.42**	**3.73**	**4.24**	**4.59**	**5.09**	**5.26**	**5.83**	**5.89**
Y3-methyl-2-isopropylphenol	0.18	1.17	1.30	1.39	1.40	1.42	1.28	1.26	1.45	1.49
Thymol	63.37	72.73	72.41	72.27	72.05	71.62	72.24	72.18	70.73	71.09
3-methyl-5-isopropylphenol	18.22	4.85	4.59	4.35	3.89	3.71	3.37	3.36	3.30	3.19
3-methyl-2-isopropylphenol	16.70	18.53	18.90	18.97	19.12	19.36	18.51	18.39	19.29	18.94
3-methyl-4-isopropylphenol	1.71	3.89	4.10	4.41	4.94	5.32	5.87	6.07	6.68	6.79
STotal.Isomer	**41.27**	**81.74**	**83.36**	**84.68**	**85.88**	**86.35**	**86.70**	**86.62**	**87.23**	**86.80**
YTotal.Isomer	10.34	30.01	31.82	31.57	28.40	26.66	21.73	20.84	21.69	21.89
Slights	3.69	1.11	1.02	0.94	0.96	0.93	0.96	0.97	0.95	1.07
Ylights	0.92	0.41	0.39	0.35	0.32	0.29	0.24	0.23	0.24	0.27
SC-10	19.53	8.95	8.19	7.57	6.79	6.50	6.06	6.06	5.32	5.36
YC-10	4.89	3.29	3.13	2.82	2.24	2.01	1.52	1.46	1.32	1.35
Sdi-isopropylated	6.15	3.25	3.05	2.84	2.28	2.09	1.64	1.62	1.76	1.86
Ydi-isopropylated	1.54	1.19	1.16	1.06	0.75	0.64	0.41	0.39	0.44	0.47
Sheavies	8.17	2.06	1.60	1.32	1.10	1.03	0.81	0.86	0.77	0.76
Yheavies	2.05	0.75	0.61	0.49	0.36	0.32	0.20	0.21	0.19	0.19
Sether	0.64	0.12	0.13	0.21	0.37	0.41	0.53	0.59	0.72	0.88
Yether	0.16	0.05	0.05	0.08	0.12	0.13	0.13	0.14	0.18	0.22

Table 0.55: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-35	PW-37	PW-39	PW-43	PW-46	PW-47	PW-48	PW-49	PW-50	PW-51
Time on Stream	60:00:07	68:00:07	81:00:06	89:00:06	93:50:06	103:44:21	104:00:21	105:00:21	106:00:21	107:00:21
Entry Temperature	93	86	93	94	94	92	92	92	92	93
Temperature	274	275	276	275	275	275	274	275	275	274
WHSV	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Guauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3
Conversion	20.90	20.08	17.84	16.40	15.83	15.10	15.45	15.77	15.28	14.40
Thymol Selectivity	61.07	61.02	60.74	60.86	61.29	60.48	59.29	59.16	59.17	58.73
Thymol Yield	12.77	12.26	10.83	9.98	9.70	9.13	9.16	9.33	9.04	8.46
S3-isopropyl-5-methylphenol	**2.73**	**2.68**	**2.60**	**2.54**	**2.52**	**2.43**	**2.51**	**2.57**	**2.45**	**2.47**
Y3-methyl-5-isopropylphenol	0.57	0.54	0.46	0.42	0.40	0.37	0.39	0.41	0.37	0.36
S4-isopropyl-3-methylphenol	**16.55**	**16.07**	**15.95**	**15.43**	**15.16**	**14.61**	**15.49**	**16.04**	**15.55**	**15.35**
Y3-methyl-4-isopropylphenol	3.46	3.23	2.84	2.53	2.40	2.21	2.39	2.53	2.38	2.21
S2-isopropyl-3-methylphenol	**6.61**	**6.75**	**6.88**	**7.10**	**7.12**	**7.65**	**7.95**	**7.86**	**8.05**	**8.16**
Y3-methyl-2-isopropylphenol	1.38	1.36	1.23	1.16	1.13	1.16	1.23	1.24	1.23	1.18
Thymol	70.23	70.52	70.49	70.83	71.19	71.01	69.55	69.08	69.42	69.33
3-methyl-5-isopropylphenol	3.14	3.10	3.02	2.95	2.92	2.85	2.95	3.01	2.88	2.91
3-methyl-2-isopropylphenol	19.04	18.57	18.50	17.95	17.61	17.16	18.17	18.73	18.25	18.12
3-methyl-4-isopropylphenol	7.60	7.81	7.99	8.26	8.27	8.98	9.33	9.18	9.45	9.64
STotal.Isomer	**86.96**	**86.53**	**86.18**	**85.92**	**86.09**	**85.18**	**85.25**	**85.64**	**85.22**	**84.70**
YTotal.Isomer	18.18	17.38	15.37	14.09	13.63	12.86	13.17	13.50	13.03	12.20
Slights	1.05	1.03	1.08	1.07	0.99	1.10	1.03	1.08	1.08	1.14
Ylights	0.22	0.21	0.19	0.17	0.16	0.17	0.16	0.17	0.17	0.16
SC-10	4.97	4.99	5.13	4.60	4.94	4.93	4.43	4.41	4.29	4.29
YC-10	1.04	1.00	0.91	0.75	0.78	0.74	0.68	0.69	0.66	0.62
Sdi-isopropylated	1.61	1.61	1.42	1.32	1.09	1.22	1.37	1.41	1.41	1.36
Ydi-isopropylated	0.34	0.32	0.25	0.22	0.17	0.18	0.21	0.22	0.22	0.20
Sheavies	0.65	0.80	0.66	1.03	0.66	0.78	0.83	0.72	0.74	0.79
Yheavies	0.14	0.16	0.12	0.17	0.10	0.12	0.13	0.11	0.11	0.11
Sether	1.05	1.17	1.29	1.46	1.50	1.84	2.20	1.94	2.30	2.51
Yether	0.22	0.23	0.23	0.24	0.24	0.28	0.34	0.31	0.35	0.36

Table 0.56: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-52	PW-53	PW-54	PW-55	PW-56	PW-57	PW-58	PW-59	PW-60	PW-61	PW-62	PW-63	PW-64	PW-65	PW-66
Time on Stream	132:00:55	133:00:55	134:00:55	135:00:55	135:54:55	152:00:55	163:14:55	179:00:55	181:00:55	182:48:55	188:00:55	188:56:55	190:00:55	191:00:55	198:04:55
Entry Temperature	92	91	92	93	94	94	96	95	95	95	89	89	90	89	90
Temperature	276	275	275	275	275	275	274	275	274	274	275	276	276	275	276
WHSV	0.72	0.72	0.72	0.72	0.72	0.3	0.3	0.3	0.3	0.3	1.2	1.2	1.2	1.2	1.2
Pump Rate (m/min)	0.12	0.12	0.12	0.12	0.12	0.05	0.05	0.05	0.05	0.05	0.2	0.2	0.2	0.2	0.2
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	15.07	15.10	14.89	14.88	13.40	27.97	28.71	27.09	26.82	27.20	7.94	7.57	6.92	6.59	5.03
Thymol Selectivity	58.98	58.49	59.56	58.44	58.75	63.17	61.47	62.94	62.84	62.46	52.94	52.78	52.07	50.10	49.89
Thymol Yield	8.89	8.83	8.87	8.70	7.87	17.67	17.65	17.05	16.85	16.99	4.20	3.99	3.60	3.30	2.51
S3-isopropyl-5-methylphenol	**2.61**	**2.57**	**2.45**	**2.52**	**2.42**	**2.91**	**2.72**	**2.63**	**2.78**	**2.82**	**2.28**	**2.34**	**2.28**	**2.19**	**2.18**
Y3-methyl-5-isopropylphenol	0.39	0.39	0.36	0.38	0.32	0.81	0.78	0.71	0.75	0.77	0.18	0.18	0.16	0.14	0.11
S4-isopropyl-3-methylphenol	**16.03**	**15.84**	**15.14**	**15.76**	**15.51**	**14.26**	**14.49**	**14.44**	**14.43**	**14.76**	**15.32**	**16.26**	**15.16**	**14.51**	**13.80**
Y3-methyl-4-isopropylphenol	2.42	2.39	2.25	2.35	2.08	3.99	4.16	3.91	3.87	4.01	1.22	1.23	1.05	0.96	0.69
S2-isopropyl-3-methylphenol	**8.00**	**8.05**	**8.21**	**8.21**	**8.28**	**6.66**	**6.53**	**6.80**	**6.91**	**6.78**	**9.36**	**9.09**	**9.13**	**8.67**	**8.97**
Y3-methyl-2-isopropylphenol	1.21	1.22	1.22	1.22	1.11	1.86	1.87	1.84	1.85	1.85	0.74	0.69	0.63	0.57	0.45
Thymol	68.88	68.85	69.77	68.81	69.14	72.61	72.14	72.50	72.26	71.94	66.26	65.59	66.21	66.39	66.67
3-methyl-5-isopropylphenol	3.05	3.03	2.87	2.97	2.85	3.35	3.20	3.03	3.20	3.25	2.86	2.91	2.90	2.90	2.92
3-methyl-2-isopropylphenol	18.73	18.65	17.74	18.55	18.26	16.39	17.00	16.63	16.60	17.00	19.18	20.21	19.28	19.23	18.44
3-methyl-4-isopropylphenol	9.34	9.47	9.62	9.67	9.74	7.65	7.66	7.84	7.94	7.81	11.71	11.29	11.61	11.48	11.98
STotal.Isomer	**85.62**	**84.96**	**85.36**	**84.94**	**84.96**	**87.00**	**85.21**	**86.82**	**86.96**	**86.83**	**79.90**	**80.47**	**78.65**	**75.46**	**74.84**
YTotal.Isomer	12.90	12.83	12.71	12.64	11.38	24.34	24.46	23.52	23.32	23.62	6.34	6.09	5.44	4.97	3.76
Slights	1.32	1.40	1.04	1.18	1.05	0.97	1.51	1.02	1.07	0.92	1.33	0.90	1.42	2.95	1.87
Ylights	0.20	0.21	0.15	0.18	0.14	0.27	0.43	0.28	0.29	0.25	0.11	0.07	0.10	0.19	0.09
SC-10	4.20	4.20	4.25	4.13	3.96	4.97	4.79	4.81	4.76	4.88	3.29	3.37	3.35	3.76	3.12
YC-10	0.63	0.63	0.63	0.62	0.53	1.39	1.38	1.30	1.28	1.33	0.26	0.25	0.23	0.25	0.16
Sdi-isopropylated	1.41	1.50	1.35	1.44	1.32	2.26	2.47	2.22	2.20	2.26	1.00	0.92	0.91	0.79	0.63
Ydi-isopropylated	0.21	0.23	0.20	0.21	0.18	0.63	0.71	0.60	0.59	0.61	0.08	0.07	0.06	0.05	0.03
Sheavies	0.66	0.92	0.85	0.96	0.81	0.72	0.99	0.81	0.73	0.84	0.87	0.72	0.94	0.68	0.81
Yheavies	0.10	0.14	0.13	0.14	0.11	0.20	0.28	0.22	0.20	0.23	0.07	0.05	0.06	0.04	0.04
Sether	1.95	2.10	2.15	2.29	2.36	0.79	0.87	0.86	0.85	0.82	4.83	4.54	4.85	4.94	5.03
Yether	0.29	0.32	0.32	0.34	0.32	0.22	0.25	0.23	0.23	0.22	0.38	0.34	0.34	0.33	0.25

Table 0.57: Conversion, selectivity and yield data for H-MFI-90 powder repeat (cont.)

	PW-67	PW-68	PW-69	PW-70	PW-71	PW-72	PW-73	PW-74	PW-75	PW-76	PW-77	PW-78
Time on Stream	201:00:55	201:30:55	201:58:55	205:00:55	205:30:55	206:00:55	206:30:55	232:10:55	233:30:55	236:32:55	238:30:55	246:36:55
Entry Temperature	90	90	89	85	85	85	85	93	93	92	92	90
Temperature	274	275	275	275	275	275	275	274	275	275	275	275
WHSV	1.81	1.81	1.81	3.62	3.62	3.62	3.62	0.96	0.96	0.96	0.96	0.96
Pump Rate (m/min)	0.302	0.302	0.302	0.604	0.604	0.604	0.604	0.16	0.16	0.16	0.16	0.16
Gauge Pressure (bar)	2	2	2	2	2	2	2	2	2	2	2	2
Absolute Pressure (bar)	3	3	3	3	3	3	3	3	3	3	3	3
Conversion	2.60	2.47	2.42	1.36	0.81	0.92	0.94	1.33	1.41	1.37	1.34	1.25
Thymol Selectivity	34.18	32.36	32.29	3.14	4.53	3.94	3.48	11.19	9.96	10.82	9.89	10.31
Thymol Yield	0.89	0.80	0.78	0.04	0.04	0.04	0.03	0.15	0.14	0.15	0.13	0.13
S3-isopropyl-5-methylphenol	**1.65**	**1.55**	**1.50**	**0.32**	**0.43**	**0.29**	**0.54**	**0.86**	**0.89**	**0.42**	**0.73**	**0.72**
Y3-methyl-5-isopropylphenol	0.04	0.04	0.04	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
S4-isopropyl-3-methylphenol	**9.92**	**9.57**	**9.55**	**1.01**	**1.59**	**1.30**	**1.50**	**3.24**	**2.94**	**2.76**	**2.61**	**3.15**
Y3-methyl-4-isopropylphenol	0.26	0.24	0.23	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04
S2-isopropyl-3-methylphenol	**7.12**	**6.58**	**6.76**	**1.38**	**2.22**	**2.11**	**1.82**	**6.63**	**6.20**	**6.47**	**5.78**	**6.17**
Y3-methyl-2-isopropylphenol	0.18	0.16	0.16	0.02	0.02	0.02	0.02	0.09	0.09	0.09	0.08	0.08
Thymol	64.65	64.65	64.45	53.64	51.65	51.57	47.45	51.02	49.84	52.87	52.03	50.67
3-methyl-5-isopropylphenol	3.11	3.11	3.00	5.45	4.95	3.77	7.30	3.93	4.47	2.03	3.83	3.53
3-methyl-2-isopropylphenol	18.77	19.11	19.06	17.27	18.13	16.98	20.44	14.79	14.70	13.49	13.74	15.47
3-methyl-4-isopropylphenol	13.47	13.14	13.49	23.64	25.27	27.67	24.82	30.26	30.99	31.61	30.41	30.33
STotal.Isomer	**52.86**	**50.06**	**50.11**	**5.85**	**8.77**	**7.63**	**7.33**	**21.93**	**19.99**	**20.46**	**19.02**	**20.36**
YTotal.Isomer	1.37	1.24	1.21	0.08	0.07	0.07	0.07	0.29	0.28	0.28	0.25	0.26
Slights	2.94	3.32	3.26	5.64	9.96	8.37	8.49	5.58	5.49	5.75	5.74	5.82
Ylights	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.07	0.08	0.08	0.08	0.07
SC-10	1.65	1.54	1.51	-	-	-	-	-	-	-	-	-
YC-10	0.04	0.04	0.04	-	-	-	-	-	-	-	-	-
Sdi-isopropylated	0.26	0.26	0.20	-	-	-	-	0.29	0.29	0.32	0.33	0.36
Ydi-isopropylated	0.01	0.01	0.00	-	-	-	-	0.00	0.00	0.00	0.00	0.00
Sheavies	1.16	1.35	1.05	4.57	4.29	4.06	4.64	1.99	4.62	2.82	3.13	1.68
Yheavies	0.03	0.03	0.03	0.06	0.03	0.04	0.04	0.03	0.06	0.04	0.04	0.02
Sether	15.08	16.02	15.78	5.36	7.33	6.85	7.25	19.11	22.12	21.19	20.45	17.46
Yether	0.39	0.40	0.38	0.07	0.06	0.06	0.07	0.25	0.31	0.29	0.27	0.22