

Re-coding of UCTPHO and UCTOLD in Visual Basic for Applications

RE-SUBMISSION AFTER EVALUATION

23 November 2016

University of Cape Town

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Declaration

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Signed by candidate

GERARD DE SWARDT
20 July 2016

EXECUTIVE SUMMARY

UCTOLD, IAWPRC and UCTPHO are activated sludge system diurnal simulation software programs written and compiled in TurboPascal 3.1 by the Water Research Group at the University of Cape Town in the late 1980s and early 1990s. IAWPRC is identical to International Water Association (IWA) Activated sludge Model No 1 (ASM1, Henze et al., 1987) and UCTOLD is an earlier variation of ASM1 that makes no material difference to simulation results when each are run with their default parameters – the difference is explained by Dold and Marais (1985). Details on the use of UCTOLD and IAWPRC was published by Dold et al. (1991) and this guide remains essential reading for the responsible use of the recoded UCTOLD and UCTPHO presented in this thesis.

In the early 1990s, when the kinetics of phosphorus accumulating organisms (PAO) were sufficiently well understood, biological excess P removal (BEPR) was added to UCTOLD to yield UCTPHO. This software has the same look and feel as UCTOLD/IAWPRC and so a guide for it was never published. Details of the BEPR research that was codified into it are given by Wentzel et al. (1991) and Clayton et al. (1991). Later, much of the Wentzel BEPR model was integrated into ASM1 to form ASM2 (Henze et al., 1995). So UCTPHO and ASM2 differ in the same way as UCTOLD and ASM1/IAWPRC differ, essentially only in the fate of the product of the hydrolysis of slowly biodegradable particulate organics (BPO) – in ASM1/2, this product enters the bulk liquid as readily biodegradable soluble organics (BSO) with the ordinary heterotrophic organisms (OHO) utilizing only BSO, whereas in UCTOLD/UCTPHO the BPO product is utilized directly by the OHO and so does not enter the bulk liquid (Dold and Marais, 1985).

One aspect is very important to note about the models embedded in these codes – UCTOLD and ASM1 are only for biological N removal systems and UCTPHO and ASM2 are only for biological N and P removal systems. One cannot simulate a N and P removal system with UCTOLD (or ASM1) and one cannot simulate a N removal system only with UCTPHO (or ASM2). The kinetics of denitrification in UCTOLD/ASM1 and UCTPHO/ASM2 are not the same - the details of the differences are explained by Clayton et al. (1991).

For two decades up to around 2010, UCTOLD and UCTPHO provided free activated sludge system simulation tools to consultants, municipalities and operators to predict the performance of the activated sludge systems of wastewater treatment plants. Therefore smaller consultancies had the software available for use without requiring expensive commercial software for the modelling of household/municipal wastewater.

With the advancement of computer hardware and Windows operating systems over two decades, the UCTOLD and UCTPHO software (not the models coded within them) grew outdated and gradually lost functionality. Then when 64 bit processor personal computers (PC) became available, the old compiled TurboPascal 3.1 software could no longer be run – they can still run on 32 bit processor WinXP PCs. Re-coding the software was therefore required if the continued use of the software were to be ensured. This recoding into Excel/VBA was undertaken in this thesis.

Some considerable effort also went into the improvement of the user interface. The new interface allows quick input and configuration of the biological reactors of the activated sludge system, and the recycle streams.

Several challenges presented themselves during the recoding stage of the project, most notable of which were the data management structures and the calculation time minimisation. Also, significant time was also spent on simulations to determine the effects of the integration parameters on calculation time, and to determine how to minimise the calculation time. After struggling with these challenges for some months, the recoded programs started to present results similar to the original TurboPascal compiled code, about a year after commencement with the project.

This Beta version has the same functionality that the original Turbo Pascal versions had including Adjustment of the Wastage Pattern and Graphical Display of Diurnal Results. The calculation of activated sludge ISS concentration was added as an option by including the influent OHO and PAO ISS to determine reactor TSS concentration for N and N&P removal systems using results from Ekama and Wentzel (2004). So, instead of having to enter an activated sludge VSS/TSS ratio, the option to calculate it from entered influent VSS and TSS data can now be selected to calculate the reactor TSS concentration.

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LIST OF ACRONYMS

AD	Anaerobic Digestion
ADWF	Average Dry Weather Flow
AS	Activated Sludge
ASM	Activated Sludge Model
HP	Hewlett Packard
JHB	Johannesburg
MLE	Modified Ludzack-Ettinger
MOC	Minimum Output Concentration
OUR	Oxygen Utilization Rate
PWSSD	Plant Wide Steady State Model
RAS	Return Activated Sludge
TP	Turbo Pascal
UCT	University of Cape Town
VB	Visual Basic
VBA	Visual Basic for Applications
WAS	Waste Activated Sludge
WRC	Water Research Commission
WW	Wastewater
WWTP	Wastewater Treatment Plant

1. INTRODUCTION

UCTOLD, IAWPRC and UCTPHO are activated sludge system diurnal simulation software programs written and compiled in TurboPascal 3.1 by the Water Research Group at the University of Cape Town in the late 1980s and early 1990s. IAWPRC is identical to International Water Association (IWA) Activated sludge Model No 1 (ASM1, Henze et al., 1987) and UCTOLD is an earlier variation of ASM1 that makes no material difference to simulation results when each are run with their default parameters. UCTOLD and IAWPRC/ASM1 differ only in the fate of the product of the hydrolysis of slowly biodegradable particulate organics (BPO) – in ASM1, this product enters the bulk liquid as readily biodegradable soluble organics (BSO) with the ordinary heterotrophic organisms (OHO) utilizing only BSO, whereas in UCTOLD, the BPO product is utilized directly by the OHO and so does not enter the bulk liquid – the details of the difference is explained by Dold and Marais (1985). A guide on the use of UCTOLD and IAWPRC was published by Dold et al. (1991) and this guide remains essential reading for the responsible use of also the recoded UCTOLD and UCTPHO presented in this thesis.

In the early 1990s, when the kinetics of phosphorus accumulating organisms (PAO) were sufficiently well understood, biological excess P removal (BEPR) was added to UCTOLD to yield UCTPHO. This software has the same look and feel as UCTOLD/IAWPRC and so a guide for it was never published. The details of the BEPR research that was codified into it are given by Wentzel et al. (1991) and Clayton et al. (1991). Later, much of the Wentzel BEPR model was integrated into ASM1 to form ASM2 (Henze et al., 1995). So UCTPHO and ASM2 differ in the same way as UCTOLD and ASM1/IAWPRC differ.

One aspect is very important to note about the bioprocess models embedded in these codes – UCTOLD and ASM1 are only for biological N removal systems and UCTPHO and ASM2 are only for biological N and P removal systems. One cannot simulate a N&P removal system with UCTOLD (or ASM1) and likewise one cannot simulate a N removal system only with UCTPHO (or ASM2). The kinetics of denitrification in UCTOLD/ASM1 and UCTPHO/ASM2 are not the same. The difference hinges around the reduction factor for the hydrolysis/utilization of BPO for anoxic conditions relative to aerobic conditions (η_g) – in UCTOLD/ASM1 it is 0.33 and in UCTPHO/ASM2 it is 0.66. The details of the differences are explained by Clayton et al. (1991).

For two decades up to around 2010, UCTOLD and UCTPHO provided free activated sludge system simulation tools to consultants, municipalities and operators to predict the performance of the activated sludge systems of wastewater treatment plants. Therefore, smaller consultancies had the software available for use without requiring expensive commercial software for the modelling of household/municipal wastewater.

With the advancement of computer hardware and Windows operating systems over two decades from 1990 to 2010, the UCTOLD and UCTPHO software (not the models coded within them) grew outdated and gradually lost functionality. First, the print and screen graphics functions stopped working. Then when 64 bit processor personal computers (PC) became available, the old compiled TurboPascal 3.1 software could no longer be run – the last PC it can still run on were 32 bit processor WinXP PCs. Therefore re-coding the software was

required if the continued use of the software is to be ensured. This recoding into Excel/VBA was undertaken in this thesis.

The characteristics and performance of the original UCTOLD was reported in 1991 as follows as explained by Dold et al. (1991):

1.1. Limitations

The program can be used to predict the response of single or in-series completely mixed reactor systems with or without inter-reactor recycles (recycles opposite to the direction of flow through the system) over the range of temperatures from 14 to 22 degrees C. The reactors may be aerated or unaerated and the sludge age may vary from 2 to 30 days. Waste flow and/ or loads may be steady or cyclic.

1.2. Performance

The performance of UCTOLD and IAWPRC were considered in 1991 and the following reference was made to the performance of IAWPRC on a 10-MHz IBM AT with a square wave influent loading pattern for a two-reactor system (Page 3.3, Dold et al. (1991)):

1.2.1. Steady state simulation

The simulation duration was 18 seconds

1.2.2. Diurnal simulation

It took 10 minutes to reach a dynamic solution over five 24 hour cycles, i.e. 1 minute per cycle per reactor.

This performance is compared with the measured performance of the re-coded VBA software later in this document, where comparable results are achieved.

2. AIM OF THE PROJECT

This project aims to continue providing a free tool to users requiring a modelling facility for municipal wastewater. The re-coded software is intended to be used in the following applications:

2.1. Stand-alone package

The program can be used as a stand-alone package to model the wastewater quality through the reactors when the reactor sizes are known.

The dynamic modelling capability of UCTPHO and UCTOLD is summarised as follows (Wu and Ekama, 2015):

In dynamic AS models, such as ASM1 (Henze et al., 1987) and ASM2 (Henze et al., 1995), the state of completion of the bioprocesses is time dependent. Thus dynamic AS models are useful to evaluate and predict the time dependent response of the treatment system (Ekama & Wentzel, 2008a); however, they are not always utilised correctly. Dynamic models comprise of “numerous internal interactions between state variables and dynamic behaviour of input variables and local conditions” (Makinia, 2010: 57) and require a high-level of input information such as reactor volumes, initial reactor concentrations, inter-connecting flow rates, influent wastewater characteristics, and kinetic and stoichiometric parameters (Ekama, 2009). As such, they are structured for the optimisation of WWTP’s rather than for system sizing and overall system design (van Haandel & van der Lubbe, 2007; Ekama, 2009). Using dynamic AS models for this purpose will result in the main problem losing focus and a case of trial and error for system design (Ekama, 2009). This can be brought about by the user-friendly interfaces of the current AS simulation software, which easily covers the gaps in the knowledge and understanding of the dynamic models (Ekama, 2009; Hug et al., 2009). Dynamic AS models, however useful they are, do not always provide the necessary information and at times can be too complicated for the design task. A firm understanding of the models is required for responsible and effective modelling, which is more than only knowing where the start simulation button is located.

The Excel/ VBA structure of the UCTPHO UCTOLD program is as follows:

The complete original Turbo Pascal 3.1 coding was translated into VBA with the exception of the input and output handling. All inputs and outputs are stored on Excel sheets, which would enable the easy merging of PWSSD model and UCTPHO UCTOLD and the simplest form would be for PWSSD to write the required inputs for UCTPHO UCTOLD to the required Excel Sheets, including the reactor sizes with recycle rates and operational arrangements. Following this, the steady state and diurnal simulations can be performed by UCTPHO UCTOLD.

2.2. Add-on to PWSSD

The intention is that this program will be used as a “clip-on” to the recently completed PWSSD VBA project (Wu and Ekama, 2005), which is a Plant Wide Steady State Design.

The Project presented in this thesis will provide the functionality of dynamic modelling of the activated sludge in the plant to the plant wide steady state model design.

The detailed description of the PWSSD project is provided in the following abstract (Wu and Ekama, 2005):

Models are used as prognostic and diagnostic tools in order to design, analyse, and optimise biological and physical treatment processes in a WWTP. With steady-state WWTP models, high-level answers are found efficiently with explicit algebraic equations and low level of input information. These models can size the treatment system, identify main system defining parameters, and generate the overall WWTP scheme and initial conditions for dynamic simulation. Hence, they are powerful standalone tools and useful pre-processors to improve the reliability of dynamic models. In recognition of their value, a Plant-Wide Steady-State Design and Analysis (PWSSD) program was developed within the Excel/VBA environment. The PWSSD program integrates various steady-state models with an expert guided user-interface that provides systematic assisted interaction and exploration of the steady-state models. The program caters for commonly used AS configurations (MLE, JHB, and UCT) and important biological and non-biological unit processes, such as flow balancing, primary and secondary settling, mechanical surface aeration, and anaerobic (AD) sludge digestion such of primary sludge (PS) and waste activated sludge (WAS), either separately or blended, and anoxic-aerobic (AxAeD) digestion of WAS. Supplementing these steady-state models is a wastewater characterisation component for the characterisation of the influent WW for different data level scenarios. A capacity estimation component is also available, in which the maximum influent ADWF for a predefined WWTP can be estimated. The holistic nature of the PWSSD program allows for a plant-wide WWTP design to be completed within a few minutes, and for the generation of meaningful information that aid decision making and usage of dynamic simulation software. The program was developed with a flexible structure and additional models and design tools are planned for future editions of the program.

The Excel/ VBA structure of this PWSSD program is as follows (Wu and Ekama, 2015):

The user-interface component was developed in Visual Basic for Applications (VBA), and the data storage and model computation components were developed using spreadsheets and VBA code. In short, the program can be described as a spreadsheet based application. VBA is a subset of Visual Basic (VB); there are some differences between the two, but the overall structure of VBA and its functionalities are similar to VB. VBA requires a host application, which in this case is Microsoft Excel. A host application is an application that contains and runs an application within itself, i.e. the PWSSD program is not a standalone program and cannot run outside of the Excel environment. The foremost advantage of this structure is that it allows the hosted program (in this case the PWSSD program) to inherit the core functions of the host application (Excel). VBA is therefore typically used to supplement Excel spreadsheets or projects developed in the Excel (and Microsoft Office) environment. The PWSSD program was developed on the 32-bit Excel 2010 version; however, it is compatible

on both 32-bit and 64-bit Excel 2010 and 2013 (although the 2010 version is recommended). The PWSSD program has not been tested on different regions of Excel; incompatibilities may arise on a non-English version of Excel.

3. SOFTWARE SELECTION

The selection of modern software, for the continued use and preservation of the software developed at UCT, presented the first challenge.

At first it was considered to use Modelica to make use of its process oriented features, but since this software is not widely in use in South Africa, support and training would have added to the challenge instead of contributing towards the solution.

It was then decided to do the coding in VBA Excel since most engineers are familiar with the use of Excel and the PWSSD was already being coded in VBA.

The project was undertaken on:

- Windows 7
- MS Office 2010
- 64 bit computer (i7 HP EliteBook 8570p)

4. CODING PROJECT

The re-coding involved the basic conversion of syntax as well as more complex data handling and the interface design for the new program.

4.1. Conversion from TP to VBA

The conversion of code from Turbo Pascal to Visual Basic for Applications generally requires the following:

4.2. Syntax

The general changes that can be applied directly to the syntax of the Turbo Pascal code are as follows:

Turbo Pascal	Visual Basic for Applications
:=	=
Procedure	Sub
;	not applicable
[]	()
}	'
begin;	not applicable

end;	end sub or end if
------	-------------------

4.3. Structure

Nested procedures, occurring in Turbo Pascal, are not supported in VBA. Therefore all procedures occurring within another procedure has to be removed and turned into a stand-alone procedure (sub).

The implication of this is that all the variable declarations need to be checked and/or changed to global variables or the variables have to be declared in each of the procedures. This could lead to some challenges with respect to the use of values of variables and determining whether the latest calculated values are transferred correctly.

4.4. User interface design

The user interface was designed with the aim to create an easy transition for users of the previous TP version, but with additional ease of use by saving the existing project information for use at start-up of the next session. The aim of this is to reduce the time spent on data entry between simulations and allow rapid setting up of projects for simulations.

Refer to the User Guide in Annexure A (2.1) for further information.

4.4.1. Design dashboard

The TP version included a start-up dashboard from where all the program steps were accessed and progress could be followed, but this process was not user friendly to the extent of Windows software and therefore the Windows based environment offers a significant improvement to the interface design.

The design dashboard at start-up in the new VBA version is the main menu, from where all program actions or sub menus are accessed. This menu also allows the user to select the model to be used in the simulations i.e. UCTPHO or UCTOLD and what data input would be used i.e. Steady State or Diurnal. All user interactions that are required, are accessed in the frame "Process Model".

The seven main menu actions must be selected in sequence as was the case in the TP version and the tick box next to each button will indicate whether that part of the input information or constants have already been specified or not. If not, the user will not be allowed to proceed or continue with the next step.

The remainder of the main menu is taken up by a multipage display which allows the user to select either the flow diagram of the selected process configuration or the calculation status of the steady state calculation, which displays convergence and timing of this calculation. This display was very useful during debugging and was retained since the long calculation times leave the user in the dark as to whether convergence could be expected or not, and the display gives an indication whether the process should be aborted due to non convergence.

4.4.2. Sub-menu user inputs

All user inputs in the sub-menus are done in a similar way to the main menu, but default values or values from the previous project are displayed. All parameters can be changed in these sub-menus and where program defaults must be restored, default option buttons are included in the sub-menus.

The sub-menus were designed as separate design dashboards per section as set out in the original TP version, with all reverting back to the Main Menu after completion. The submenus are as follows:

- Wastewater Composition
- Process Configuration
- Process Operation
- Kinetic Constants
- Stoichiometric Constants
- Steady State Simulation
- Diurnal Simulation

4.4.3. Output data interface

The output data is displayed on display screens (forms) and also written to Excel sheets. The Excel sheets will make copying and printing of results easy after completion of a simulation.

4.4.4. Graphical results

All diurnal graphs that the user selects will be stored under the folder "OutputGIF" that is created for this purpose until the next time a simulation is started, at which time all the files in this folder are deleted.

4.5. Project design life cycle

The following have to be included in a software design project:

4.5.1. Analysis of user requirements

The requirements of the users are to be able to use the software for the modelling of biological treatment systems for the treatment domestic wastewater without the need for a long and challenging software training period. Therefore the software must be user friendly and contain simplified inputs for the quick setup of the most common process configurations that will generally be encountered in municipal wastewater treatment plants.

4.5.2. Program design

VBA lends itself to a user friendly software design with the availability of user forms for the creation of a functional user interface. This project made use of this feature to create a user friendly input mechanism while calculations are still being done with the re-coded version of the original TP code translated into VBA code.

4.5.3. Program coding

The VBA re-coding was initially done for UCTPHO until the code became functional.

Only at this point, the compared TP code between UCTPHO and UCTOLD (Excel tab “UCTPHO and UCTOLD Pascal code”) highlighted the differences for which IF statements were introduced to differentiate between the two models.

This reduced the duplication of work and left clear boundaries between the code of the UCTPHO and UCTOLD programs, that are simple to follow in the various modules where differences are managed.

The major differences are:

- Difference in default parameter values as seen in Annexure B: Default Constants, comparing constant values in UCTPHO and UCTOLD (Differences are shown in bold text)
- Procedures dealing with P removal were included for UCTPHO after the development of UCTOLD in the original development of the software

4.5.4. Operating and maintaining the system

The system will be maintained and improved to remove “bugs” reported by users to gerard.deswardt@mottmac.com.

4.6. Declaration of variables

All the variables had to be declared in the relevant types to be similar in VBA as per the original Turbo Pascal code.

4.7. Declaration of types

All the custom user types could be declared in VBA similar to TP except the following dynamic array types:

- $nbyn = \text{array}[\text{subs}]$ of $\wedge n\text{vector}$: a one dimensional array of pointer to one dimensional vectors (providing two dimensional matrix) is used in the calculation of the steady state matrix. The creation of a class module, “clsNbynType”, provided the solution to this problem.
- Type $\wedge diarray$ (pointer in turbo pascal) had to be defined – VBA does not make use of pointers, or if so, it is not simple to achieve. However, eventually the creation of a class module clsPointerDIarray proved to solve this problem.

VBA supports variable size arrays via the Redim (re-dimension) statement. This might have provided a simpler, standard solution.

4.8. Input/ Output Management

The program has been designed to handle data separately for input, calculations and output.

4.8.1. Location of Input Data

All the project input data is stored on Sheet “InputData”. This includes the diurnal or steady state wastewater flow and quality data as well as the raw and settled wastewater fractions, the process configuration with recycle flow specification for the various recycles.

The default and custom Kinetic and Stoichoimetric constants are stored on tab “Parameters”.

4.8.2. Location of Output Data

The output data is stored on the following sheets:

- Steady State output on “OutputSS”
- Diurnal response on “DIResponse”
- Diurnal output on “OutputDI”
- Diurnal data points of all compounds over the 24 hour cycle on “GraphicOutput”

These sheets could be printed from Excel after exiting the program.

4.8.3. Printing

No provision is made for printing of data or results, but the data is stored on Excel sheets and could be manipulated from there, including printing.

4.8.4. Methods of data input

Data can be entered directly into the Sheet “InputData” before initiation of the program or via the Data Input Menu after initiation of the program. This also applies to the editing of the data.

4.9. VBA Structure

The VBA structure consists of Userforms, Modules and Class Modules. The various occurrences of each of these are listed below.

The Userforms are the menu screens of the user interface. Each button on such a userform is supported by code to be executed when the button is clicked.

The following Userforms are found in the program:

4.9.1. frmASP_Main

This menu presents the main interface and all actions completed lead to reverting back to this screen.

4.9.2. frmAbout

Information is provided about this software and its history.

4.9.3. frmDataMenu

The data menu allows data input either as diurnal data or steady state data input. The wastewater fractions also have to be accepted or entered here, as well as the influent water alkalinity.

4.9.4. frmFractions

This menu is initiated from frmDataMenu and allows the selection of either default or changed values of raw or settled wastewater fractions.

- 4.9.5. ProcessConfiguration
- The process configuration can be selected here from some options or a custom process entered. The recycle rates/ ratios need to be specified and the aeration state of each reactor.
- 4.9.6. ProcessOperation
- The process operating parameters are specified here. This includes the sludge age and temperature, but the recycles could also be adjusted here.
- 4.9.7. frmKineticMenu
- The default values of the kinetic constants could be accepted here or new values could be entered.
- 4.9.8. frmStoichMenu
- The default values of the stoichiometric constants could be accepted here or new values could be entered.
- 4.9.9. frmSteadySimMenu
- The steady State State Simulation is initiated from this form.
- 4.9.10. frmDiurnalSimMenu
- This menu initiates the Diurnal Simulation after the integration parameters have been adjusted. The button “Graphical Output” call up the screen “frmGraphicDisplay”. The button ”Wastage Pattern” opens the screen “frmOutputWaste”.
- 4.9.11. frmDisplayResults
- The results from the Steady State Simulation are displayed on the form, followed by the results from the Diurnal Simulation if this is also executed.
- 4.9.12. frmGraphicDisplay
- The form displays graphs of the diurnal results per compound for a selected reactor.
- 4.9.13. frmOutputWaste
- The button ”Wastage Pattern” allows the on and off switching of wastage during the diurnal intervals.

4.10. Calculation code/ Modules

This project dealt with the re-coding of Turbo Pascal code into VBA and therefore all calculations are performed directly in the VBA code i.e. no calculations are performed in the Excel sheets.

The program consists of the following Modules:

4.10.1. mdlCaptions

This module contains the captions for each compound, process, constant and unit.

4.10.2. mdlDisplayUnit

This module displays all outputs on the relevant output sheets when required per the selection boxes on the main menu.

4.10.3. mdlDIUnit

Diurnal unit

4.10.4. mdlExcelGauss

This module was created using the Excel matrix functions and supersedes the procedure "Gauss" due to its simplicity and improved calculation time.

4.10.5. mdlIntegrate

Integration function used by the diurnal simulation.

4.10.6. mdlKineticUnit

Entry or Confirmation of the kinetic parameters.

4.10.7. mdlMain

Initialization and starting procedures.

4.10.8. mdlNewton

Iterations of matrix calculations used in the steady state calculations.

4.10.9. mdlProcessConfiguration

Data entry for process configuration.

- 4.10.10. mdlProcessOperation
Process operation parameters.
- 4.10.11. mdlRateUnit
Calculation of process rates and utilization rates.
- 4.10.12. mdlStchUnit
Entering stoichiometric constants or accepting their default values.
- 4.10.13. mdlStdyUnit
Steady state calculations.
- 4.10.14. mdlVarsUnit
Declaration of variables and user types.
- 4.10.15. mdlWasteSpecified
Enter wastewater characteristics
- 4.10.16. mdlWastePattern
This modules reads and writes the waste pattern (Sheet("InputData")), and re-calculates the wastage flows according to the adjusted pattern while keeping the mean wastage flow.
- 4.11. Class Modules
The following Class Modules have been created:
 - 4.11.1. clsNbynType
Array type for matrix in steady state calculation, used by procedure "Newton".
 - 4.11.2. clsPointerDIarray
Array type for vector used by procedure "Integrate" to determine the diurnal response.

Alternatively, the use of the Redim statement in VBA could have presented a simpler option to create dynamic arrays.

5. CODING CHALLENGES/ LIMITATIONS

The majority of TP code could be converted to VBA code without presenting major problems. However, there were a number of challenges and it took significant time to solve these problems. There were basically three challenges that deserve mentioning:

5.1. User interface

The TP code made provision for on-screen display of menus that were created using Record-type variables with multiple fields that were populated when the menu was invoked, and the selection of a menu option would be done by typing in the list number of the relevant option. Towards the end of the 1980's this was still common practice although more advanced menu programming was already in use.

In the Windows environment the users have become familiar with a more user friendly interface and it would be expected from this program to provide a modern interface with improved input and output management. VBA lent itself to the task with the ease of creating userforms for menu displays and this improved the selection/ change of constants and other parameters. More information is available in Annexure A: User Manual.

5.2. Data management

The challenge presented in the original Turbo Pascal code was to create dynamic variables for dynamically declared matrix sizes, which are dependent on the number of reactors, each having to deal with all the compounds and processes in the reactions.

These matrixes then become very large and to limit the memory utilisation by the program, the use of dynamically declared variables become essential. This is done in Turbo Pascal by the use of Pointers, and the alternative that was successfully incorporated into the VBA version, was the creation of class modules, which could be dynamically declared to serve a similar purpose. Alternatively, the use of the Redim statement in VBA could have presented a simpler option to create dynamic arrays.

This re-coding of the pointers presented a major challenge since VBA does not allow this programming style, so an alternative needed to be found to manage the high volume of data.

The purpose of pointers is to dynamically create variables as required during program execution in order to minimize the memory use. Therefore it aims to create matrices of just the required size, which in turn would speed up all the calculations following

the sizing of the matrices due to the elimination of excessive sized matrices. Alternatively a fixed size matrix could have been created as well as the number of matrices, both to the maximum capacity of the program. This would have increased the number of calculations and therefore calculation time unnecessarily.

Eventually, this proved to provide the acceptable alternative to the pointers.

Two class modules were required:

5.2.1. clsNbynType

This Class Module is used in the procedure “sub Newton” during the steady state simulation to calculate the steady state matrix (Jmat) with concentrations of the various compounds and

5.2.2. clsPointerDiarray

This Class Module is used during the diurnal simulation to calculate the diurnal response.

5.3. Gauss transformation

The re-writing of the original code for the integration during the diurnal simulation could not be converted successfully, especially the Gauss transformation (mdlGauss). The following alternatives were implemented after losing so much time on trying to get the code to work:

5.3.1. Alternative Gauss Code (mdlGaussianElimination)

VBA Gauss code was obtained by a Google search off the internet. This code was first tested with simple matrices and then converted and subsequently incorporated into the program.

When it was found that this code worked successfully, the calculation time was still excessive and it was felt that another alternative should be pursued i.e. using Excel matrix functions.

5.3.2. Implementing Excel Functions (mdlExcelGauss)

It was decided to make use of the Excel matrix functions, using the Identity Matrix instead of the Gauss procedure to determine the values of the variables. This was successfully done and it also reduced the calculation time.

5.3.3. Convergence in loop: sub Newton

This procedure calculates the Gauss Elimination and tests convergence of a test parameter after each Inversion. This parameter could not be found to converge. For this reason, an alternative test parameter was introduced and this tests for convergence of parameter 1 in reactor 1 within an accuracy limit of 0.001. This produced satisfactory results compared to the TP versions of the software.

However, MaxF determines the maximum difference in the MassRateIn between iterations for all reactors and all compounds, so ideally this parameter must be made to converge in order to achieve a mass balance. Up to now, this has been a major challenge which has not been successfully solved.

5.4. Other challenges

There were several other challenges in the programming, of which a few are mentioned as follows:

5.4.1. Code discrepancies

There were several instances of discrepancies in the code where some variables were missing and new variables had to be declared to restore the functionality of the relevant procedures (subs in VBA). The reasons for the discrepancies were not clear, but may have been due to the differences in variable declaration in TP and VBA. Also, some internal Borland functions, declarations and their purpose were unknown such as the declarations at the beginning of modules:

- Interface: Section headings in a Pascal 'Unit', which is somewhat similar to a VBA 'class'
- implementation: These are drivers for various graphics cards that used to be found on PCs.
- procedure ATTDriverProc;
- procedure CgaDriverProc;
- procedure EgaVgaDriverProc;
- procedure HercDriverProc;
- procedure PC3270DriverProc;

The declaration of new variables generally turned out to be successful after careful consideration of where the declarations had to be made and whether local or global variables had to be declared.

5.4.2. VSS and TSS Calculation

5.4.2.1. Original TP calculation

AS models only work in COD, N and P mass balances. To convert organic solids concentrations from COD to VSS, a COD/VSS ratio is used. The same COD/VSS ratio (entered with the stoichiometric coefficients) is used for all the organics solids components, viz (1) the influent unbiodegradable particulate organics (UPO), (2) & (3) the endogenous residue of the OHO and PAO and (4) & (5) OHO and PAO biomass itself. In Wu and Ekama's (2014) PWSSD model it is possible to assign a different COD/VSS ratio to the UPO (2) than the other four (2 to 5). This may lead to different results between PWSSD and the recoded UCTOLD and UCTPHO. This is an aspect that will be fixed in future editions of UCTOLD and UCTPHO.

Also, in the TP versions of UCTOLD and UCTPHO, the activated sludge VSS/TSS ratio is an input and is used in all VSS/TSS calculations.

The concentrations of the following particulate compounds are calculated:

1	Zbh (hetero.)	g COD m-3
2	Zba (auto.)	g COD m-3
3	Zbg (polyP org.)	g COD m-3
4	Ze (endog. COD)	g COD m-3
5	Zi (inert. COD)	g COD m-3
6	Sads (adsorbed COD)	g COD m-3
7	Senm (enmeshed COD)	g COD m-3
8	Sphb (PHB COD)	g COD m-3
9	Nobp (prt bio N)	g N m-3
10	Ppp (stored polyP)	g P m-3

Compounds 1-8 are used to determine the VSS i.e. the concentrations added and divided by the COD/VSS ratio (default value 1.48) to convert the figure to VSS units. For UCTOLD, the P related concentrations i.e. compounds 3 and 8 will be zero.

In the old TP code, once the VSS concentration is known, the TSS is calculated by dividing the VSS by the activated sludge VSS/TSS ratio that was specified as an input (Raw VSS/TSS default = 0.75, Settled=0.83).

Some discrepancies noted in the VSS calculation between the new VBA code and the original TP code are due to a minor calculation error in the TP code of UCTPHO, which only calculates the VSS from compounds 1-6 instead of 1-8. This was likely due to the conversion from UCTOLD, which calculated the VSS using compounds 1-6 before these compounds were re-numbered to create UCTPHO.

5.4.2.2. New calculation option: Ekama and Wentzel (2004)

In the recoded UCTOLD and UCTPHO, the VSS/TSS option been retained to calculate the TSS concentration. For N removal systems (UCTOLD) this is acceptable but for N&P removal systems not because the polyphosphate content of the PAO has a major impact on the activated sludge VSS/TSS ratio. So instead of using a fixed input VSS/TSS ratio to be applied to all the reactors, the ISS model of Ekama and Wentzel (2004) has been added. This model was validated for both N removal (UCTOLD) and N&P removal (UCTPHO) systems.

From Ekama and Wentzel (2004), the calculation of the ISS and hence TSS (=VSS + ISS) is possible from the flux of ISS in the influent, the ISS content of the OHO (0.15 mg ISS/mg OHOVSS) and ISS content of the PAO (0.15 mg ISS/mg PAOVSS + 3.286x PP content of the PAOs). Because UCTOLD and UCTPHO work only on COD units, these stoichiometric values were converted from VSS to COD units in the new UCTOLD and UCTPHO codes presented here.

The ISS calculation is illustrated below in red where $f_{iOHO} = 0.1$ mgISS/mgCOD:

COMPOUND	UNIT	INPUT	REACTOR			Reactor 3 ISS	Calculation	
			1	2	3			
1	Zbh (hetero.)	g COD m-3	0.0	968.3	2 038.3	2 078.2	207.8	Zbh * 0.1
2	Zba (auto.)	g COD m-3	0.0	36.2	72.8	73.9	7.4	Zba * 0.1
3	Zbg (polyP org.)	g COD m-3	0.0	376.7	756.6	768.5	76.8	Zbg * 0.1
4	Ze (endog. COD)	g COD m-3	0.0	574.4	1 137.3	1 149.1		
5	Zi (inert. COD)	g COD m-3	137.6	1 062.1	1 986.6	1 986.6		
6	Sads (adsorbed COD)	g COD m-3	0.0	468.3	204.6	68.5		
7	Senm (enmeshed COD)	g COD m-3	694.1	39.8	6.0	3.5		
8	Sphb (PHB COD)	g COD m-3	0.0	82.6	49.9	27.2		
9	Nobp (prt bio N)	g N m-3	4.2	9.0	5.6	2.9		
10	Ppp (stored polyP)	g P m-3	0.0	37.7	136.1	150.9	496.0	Ppp * 3.286
11	ISSi (influent ISS)	g ISS m-3	158.9	1 226.5	2 294.2	2 294.2	2 294.2	Influent ISSi
							3 082.2	Total ISS

In order to achieve the Total ISS calculation, the modelling of the influent ISS had to be included in the system. Firstly, a means had to

be created to specify the influent ISSi and this was achieved by adding two options namely (i) entering of VSS and TSS diurnal data or (ii) entering an influent VSS/TSSi ratio.

To model the influent ISSi through the system, another parameter had to be added in the matrix calculations, of which there were originally 19 including DO. ISSi was inserted in position 11, so all compounds from 11-19 had to be re-numbered. The following changes were required:

- Changing program constants

	original	description
Public Const FirstSlow = 1		'PARTICULATE COMPOUNDS
Public Const LastSlow = 11	'10	'PARTICULATE COMPOUNDS
Public Const FirstRapid = 12	'11	'SOLUBLE COMPOUNDS
Public Const LastRapid = 19	'18	'SOLUBLE COMPOUNDS
Public Const NoPart = 11	'10	'PARTICULATE COMPOUNDS
Public Const TotalCompounds = 20	'19	'{ including DO }
Public Const LastCompound = 19	'18	
Public Const NoProcesses = 27		
Public Const NoDiVars = 24	'23	
Public Const MaxReac = 12		
Public Const MaxReacP1 = 13		'maxreac plus 1
Public Const MaxN = 248	'236	'234 changed to 236 by gds: must be >
SizeJ "{ LastCompound * (MaxReac+1) }		
Public Const NoDiurnalInts = 12		

- Re-numbering the substances in all procedures where they are used in the calculations:
 - sub SeedValues
 - sub Stoichiometry
 - sub UtilizationRates and elsewhere in mdlRateUnit
 - sub StoreResponse
 - sub DisplaySteadyState
 - sub DisplayOutputDI
 - sub DisplayDIresponse

5.4.3. Debugging

Significant time was required for de-bugging and during this process it seemed that the dynamic simulation (diurnal) was too slow because even all-night simulations did not produce realistic results.

In addition to the de-bugging itself, numerous display procedures had to be written to evaluate the output of several procedures and determine whether the procedures were functioning properly. The procedures remain in the program, but an option has been included on the

ASP_Main form to switch the writing of calculations to sheets “on” or “off”. The default is “off”. There is also a feature for switching biological processes on or off, with the sole purpose of de-bugging. This has been inactivated by setting the default value of the tick-box selected and also locking it.

After this, the simulations were operational and started producing comparable results, both in terms of predicted concentrations and run time, as the compiled DOS versions of UCTOLD and UCTPHO on 32 bit computers.

6. FUTURE WORK

Additional testing is required especially to determine the sensitivity of the accuracy parameters specified prior to model calculations. These parameters tend to determine the calculation time of simulations and may still require additional work to ensure robust calculations.

The incorporation of this software into the PWSSD (Wu and Ekama, 2015) needs to be done to utilize the capability of this software to perform diurnal simulations.

This could be easily achieved by writing the input data to the sheets “InputData” and “Parameters”. The tabs and cells that are highlighted yellow, require user input. The relevant write procedures from this project could be incorporated into the PWSSD software and modified to suit the application.

7. TESTING

Limited testing has been done and the software was run for the UCT process configuration with reasonable success to date. Calculation generally occurs successfully, but certain sensitivities have been noted:

7.1. Newton parameters (Steady State simulation)

The Minimum Output Concentration (MOC) affects the calculation time, but not proportionally to the value since the convergence of the looped calculation is affected by this.

In Section 8 it is observed that the smaller values of MOC produce better correlation with the TP version’s OUR_c (carbonaceous oxygen demand) and it is suggested that a value of 0.01 g/m³ provides acceptable level of accuracy and calculation time.

7.2. Integration parameters (Diurnal simulation)

Simple diurnal flow patterns would often lead to non convergence of the integration test variables in the code.

The results were improved by selecting values for the integration parameters i.e. % Accuracy from 0.5 to 1.0 and Theta from 0.7 to 0.8.

It was stated (Dold et al, 1991) that the reduction of %Accuracy and Theta values will increase accuracy and calculation time and it was found that these values have a significant effect on the duration of the simulation calculations.

Three integration parameters can be entered and will affect both calculation time and accuracy:

7.2.1. % Accuracy

The % Accuracy relates to a limiting value for the integration error at each step. The calculated concentration of certain parameters are compared between iteration steps. The % accuracy value is used to test for convergence between iterations.

The accuracy default is 0.5 as per the original TP code. This value could be decreased to 0.1 or even smaller to improve the accuracy, but it will lead to longer simulation times due to the more rigorous integration (See section 4.53, Dold et al. (1991)).

Due to the longer calculation times in VBA, the default value of the accuracy requirement was set at 1.0.

After completion of a diurnal simulation, the parameters could be changed and another simulation run, if required to a higher accuracy.

Although the TP default value is 0.5, the calculations are checked for convergence to values smaller than 0.001, which represents 0.1%. This will explain some minor discrepancies between results obtained from VBA code vs TP code.

7.2.2. Theta

Theta is a safety factor limit the increase in steplength from one step to the next. Default values are provided in the program. These have been found suitable for most situations, and lead to acceptably short simulation times. It is likely that most users will have no need to adjust the values. However, under certain circumstances the integration algorithm may encounter difficulties when using the default values and adjustments must be made. (Dold et al, 1991)

The theta default is 0.7 as per the original TP code. This value could be decreased to 0.6 or 0.5 to improve the performance of the integration algorithm, but it will lead to longer simulation times due to the more rigorous integration (See section 4.53, Dold et al. (1991)).

During testing however, it was found that simulations calculated faster when Theta=0.5 compared to when Theta=0.8, and therefore the VBA default was set at 0.5.

7.2.3. Integration data interval

The interval length in minutes is selected from the three options of 10, 15 and 30 minutes respectively. The default is 15 minutes and matches the default in the original TP code.

The parameter Data interval specifies the time (in minutes) between values which are stored in memory. For example, with the default Data interval of 15 minutes there will be 97 ($24/0.25 + 1$) discrete values of each parameter stored representing the response of the system over the cycle 0h00 to 24h00 per Dold et al. (1991).

The reason for reducing the Data interval to 10 minutes usually is to allow the response of rapidly-changing parameters to be tracked accurately. The penalty for reducing the Data interval is that the maximum allowable integration step length may be constrained so as to store data at the correct times where otherwise a longer step length may have been used. This will result in an increased simulation time (See section 4.54 of Dold et al. (1991)).

During testing, the interval was varied and if an interval of 30 minutes was selected, calculations were generally quicker, but this often led to a situation where convergence could not be reached while convergence was possible with a 15 minute interval.

7.3. Calculation speed improvements

On the negative side, VBA proved to produce significantly longer calculation times than the TP versions of the software on 32 bit computers. VBA also makes use of a single processor for calculations and therefore does not materialize the benefit of multiple core processors as is the case with many modern programming languages.

A number of considerations have been incorporated in an effort to improve the calculation performance:

7.3.1. Automatic calculations

The automatic calculations function in Excel is switched off at the beginning of a simulation and switched on again after completion of the simulation.

7.3.2. Screen updating

The screen updating in Excel is switched off at the beginning of a simulation and switched on again after completion of the simulation.

7.3.3. Writing calculation tables to sheets

It is an option on the main menu to write calculation tables to sheets. This causes longer calculation durations and was mainly used for debugging. This option should be switched off during normal simulations and the default value is an un-ticked box.

7.3.4. Mass balance testing

The mass balance was checked for data set 2 using UCTPHO for the process configuration previously used in the simulations. The mass balance was calculated for the steady state simulation and the a-recycle was set at 3:1.

It is desirable to add mass balances of COD, N and P as a further development. At this stage the dynamic output for a particular run was captured and TOD ($=\text{COD}+4.57*\text{TKN}$) mass balance checked, which combines COD and N and is easier to check since the actual predicted OUR and N concentrations are available for checking.

However, if the DO concentration in the aerobic reactor does not act purely as a switching function, it is suspected that the DO concentration in the a-recycle to the anoxic reactor depresses the denitrification but is not included in the OUR. This may explain why 100% COD balance is not achieved and the higher the a-recycle the lower the balance will be. Also, at low DO concentration in the aerobic reactor, there will be simultaneous nitrification-denitrification which will depress the OUR in the aerobic reactor.

Similarly, it was determined that a mass balance within 0.6% is achieved with a 1:1 a-recycle and the value changed to 2.4% for a 6:1 a-recycle.

		FOR a-recycle = 3:1								
		STEADY STATE RESULTS: UCTPHO; ISS calc: Ekama & Wentzel (2004); Inversions = 9; Calculation time = 47 seconds								
		COMPOUND	UNIT	INPUT	REACTOR			WASTE	OVERFLOW	
					1	2	3			
Particulate	1	Zbh (hetero.)	g COD m-3	0.0	1 055.8	2 218.6	2 261.5	2 261.5		
	2	Zba (auto.)	g COD m-3	0.0	40.8	82.0	83.2	83.2		
	3	Zbg (polyP org.)	g COD m-3	0.0	402.9	809.3	822.0	822.0		
	4	Ze (endog. COD)	g COD m-3	0.0	624.5	1 236.6	1 249.4	1 249.4		
	5	Zi (inert. COD)	g COD m-3	149.4	1 153.3	2 157.1	2 157.1	2 157.1		
	6	Sads (adsorbed COD)	g COD m-3	0.0	510.6	221.7	74.0	74.0		
	7	Senm (enmeshed COD)	g COD m-3	753.7	40.0	5.9	3.5	3.5		
	8	Sphb (PHB COD)	g COD m-3	0.0	88.2	53.2	28.9	28.9		
	9	Nobp (prt bio N)	g N m-3	4.8	9.9	6.1	3.2	3.2		
		9A	Noup (prt unbio N)	g N m-3	10.2	78.4	146.7	146.7	146.7	0.0
	10	Ppp (stored polyP)	g P m-3	0.0	42.2	149.3	165.2	165.2		
	10A	Pup (unbiodegradable particulate P)	g P m-3	2.1	16.1	30.2	30.2	30.2	0.0	
	11	ISSi (influent ISS)	g ISS m-3	194.1	1 498.5	2 802.9	2 802.9	2 802.9		
Soluble	12	Sbs,c (compl.RBCOD)	g COD m-3	169.6	12.0	0.1	0.0	0.0	0.0	
	13	Sbs,a (SCFA RBCOD)	g COD m-3	18.8	0.3	0.0	0.0	0.0	0.0	
	14	Na (ammonia N)	g N m-3	67.4	41.7	13.6	0.7	0.7	0.7	
	15	Nobs (sol org N)	g N m-3	4.80	0.66	1.14	1.56	1.56	1.56	
		15A	Nous (sol unbio org N)	g N m-3	2.70	2.81	2.89	2.92	2.92	2.92
	16	No3 (nitrate N)	g N m-3	0.0	0.0	6.5	17.1	17.1	17.1	
	17	Ps (soluble P)	g P m-3	17.9	51.3	17.6	0.4	0.4	0.4	
	18	Sus (sol unb COD)	g COD m-3	57.4	59.8	61.5	62.2	62.2	62.2	
	19	Alkalinity	mole m-3	10.0	8.3	6.0	4.4	4.4	4.4	
							0.0	0.0		
		Volatile SS	g VSS m-3		2 646.0	4 584.1	4 513.4	4 513.4	4 513.4	
		Total SS	g TSS m-3		4 433.0	8 188.7	8 175.8	8 175.8	8 175.8	
		OUR carbonaceous	g O2 m-3 h-1		0.0	0.0	44.5	44.5	44.5	
		OUR autotrophs	g O2 m-3 h-1		0.0	0.0	20.1	20.1	20.1	
		OUR total	g O2 m-3 h-1		0.0	0.0	64.6	64.6	64.6	
		Denit. rate	g NO3-N m-3 h-1		2.5	14.9	0.1	0.1	0.1	
		TKN	g TKN m-3 h-1		44.7	16.3	3.4	3.4	3.4	

Influent	TOD BALANCE: STEADY STATE SIMULATION							
SS1	COD CONCENTRATIONS							
SS2	COD: particulate (sum 1-8)	g/m3	903.1	3916.1	6784.5	6679.8	6679.8	0.0
SS3	COD: soluble (12,13 and 18)	g/m3	245.9	72.1	61.6	62.2	62.2	62.2
SS4	Oxygen consumed	g/m3	0.0	0.0	0.0	1068.2		
SS5	1148.9 Total COD	g/m3	1148.9	3988.2	6846.1	32377.9	6742.0	62.2
SS6	CODc BALANCE		Sti		O consumed		Sludge	
SS7	CODc in	kg COD/day	27 666.4					
SS8	CODc out	kg COD/day			12 818.0		12 809.8	
SS9	NITROGEN CONCENTRATIONS							
SS10	TKN: particulate (9)	g/m3	4.8	9.9	6.1	3.2	3.2	0.0
SS11	TKN: soluble (14, 15 AND 15A)	g/m3	74.9	45.2	17.6	5.2	5.2	5.2
SS12		Factor						
SS13	Heterotrophs: N in biomass (g/m3)	0.068	0.0	71.8	150.9	153.8	153.8	0.0
SS14	Autotrophs: N in biomass (g/m3)	0.068	0.0	2.8	5.6	5.7	5.7	0.0
SS15	PolyP organisms: N in biomass (g/m3)	0.068	0.0	27.4	55.0	55.9	55.9	0.0
SS16	N in endogenous (g/m3)	0.068	0.0	42.5	84.1	85.0	85.0	0.0
SS17	N in inert soluble (FesGn)	0.068	10.2	78.4	146.7	146.7	146.7	0.0
SS18	89.84 TKN	g/m3	89.84	277.93	466.03	455.33	455.33	5.15
SS19	TKN BALANCE		Nti		Nitrate denitrified		Sludge	
SS20	TKN in		2 163.3					
SS21	TKN out							
SS22	N flux in waste Sludge FN _s						865.1	
SS23	N flux in Effluent TKN FN _{te}						114.3	
SS24	Nitrate FN _{ne}						32.5	
SS25	Nitrate denitrified F(N _{ti} -N _{te} -N _{ne})				761.9			
SS26								
SS27	CODn BALANCE		Sti		O consumed		Sludge	
SS28	CODn in	kg COD/day	9 886.4					
SS29	CODn out	kg COD/day			-2 179.0		4 102.3	
SS30								
SS31	TOD BALANCE		Sti		O consumed		Sludge	
SS32	CODc in	kg COD/day	27 666.4					
SS33	CODn in	kg COD/day	9 886.4					
SS34	TOD in	kg COD/day	37 552.8					
SS35	CODc out	kg COD/day			12 818.0		12 809.8	
SS36	CODn out	kg COD/day			-2 179.0		4 102.3	
SS37	TOD out	kg COD/day			-2 179.0		16 912.0	
SS37	TOD MASS BALANCE		inflow Qi			waste flow Qw		over flow Qe
SS38	Flow/ reactor volume		24080	5000	2000	12000	1900	22180
SS39			m3/d	m3	m3	m3		
SS40	Rs		1	10	10	10	1	1

27 666.4 COD IN
 27 007.6 COD OUT
 -2.4% Discrepancy
 Excludes 9A-- only added in the last line
 Includes 15A

Factor from Parameters TAB
 Factor from Parameters TAB
 Factor from Parameters TAB
 Factor from Parameters TAB
 confirms Fractionation TAB or 9A

2 163.3 N IN
 2 153.5 N OUT
 865.1
 114.3
 412.2
 761.9
 -0.5% Discrepancy

9 886.4 COD IN
 9 975.7 COD OUT
 0.9% Discrepancy

37 552.8 TOD IN
 36 983.3 TOD OUT
 -1.5% Discrepancy

It is seen from this that the TOD mass balance showed a discrepancy of 1.5% across the system during the steady state simulation. The TKN balance and CODn balance were within 1.0% difference between influent and discharge while the COD balance showed a discrepancy of 2.4%. The TOD balance shows a 1.5% discrepancy, which is an acceptably well maintained balance.

8. PERFORMANCE COMPARISON: UCTPHO and UCTOLD (VBA vs TP)

The test simulations were performed for the UCT process configuration only with two alternative data sets.

8.1. Test data set 1 (default Kinetic and Stoichiometric constants accepted)

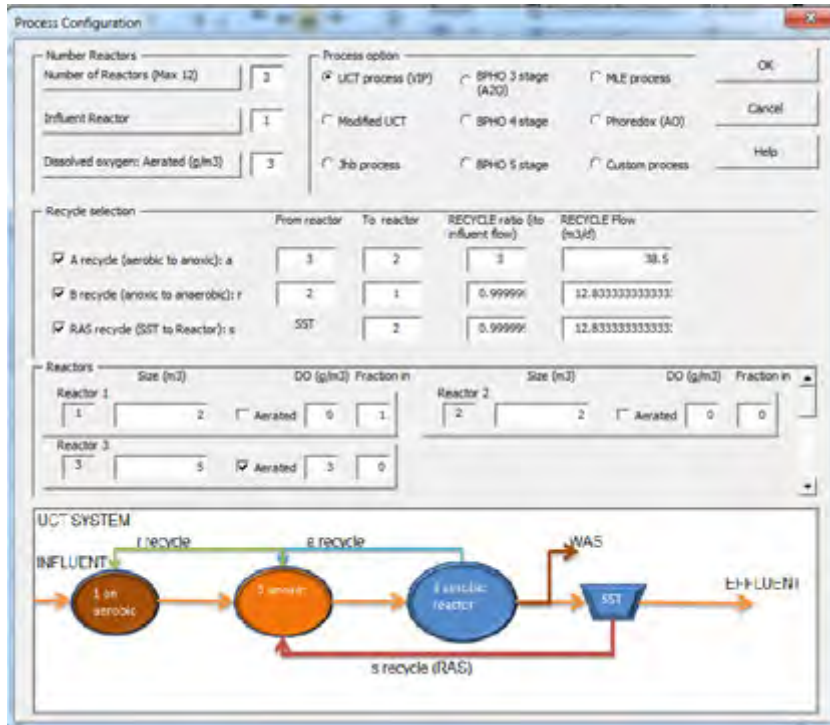
Influent wastewater

The screenshot shows the 'INFLUENT WASTEWATER DATA INPUT' dialog box. At the top, there are input fields for 'Flow rate (m³/d)', 'COD (g/m³)', 'TNV (g/m³)', 'P (g/m³)', 'VSS (g/m³)', and 'TSS (g/m³)'. Below these is a 'FLOW WEIGHTED AVERAGE (g/m³)' section. The main part of the dialog is a table for 'Diurnal flows and concentrations'. The table has columns for 'Record number', 'Time (h)', 'Flow rate', 'COD (g/m³)', 'TNV (g/m³)', 'P (g/m³)', 'VSS (g/m³)', and 'TSS (g/m³)'. The flow rate is 22 m³/d at time 0 and 0 m³/d for the rest of the day. The concentrations are constant. On the right side, there are additional options for 'Influent VSS and TSS data' and 'AS TSS Calc'.

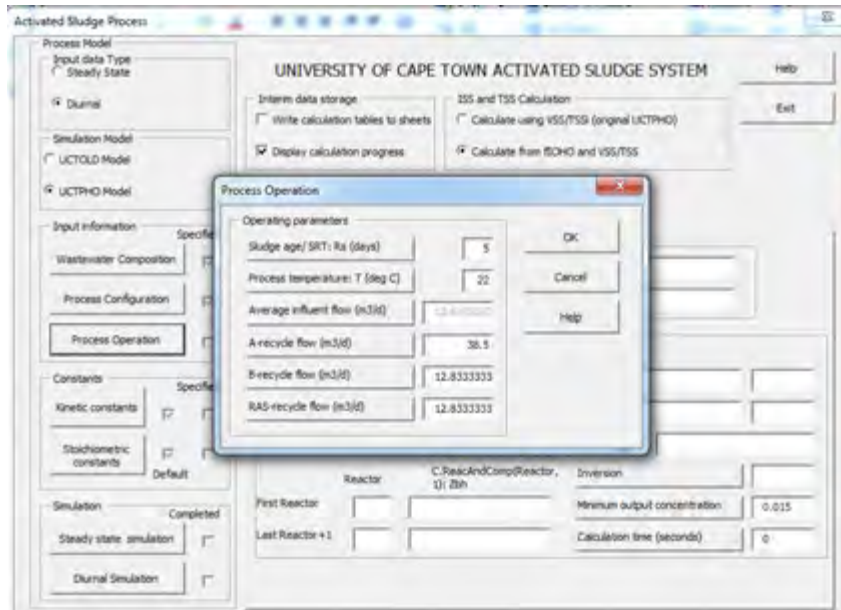
Record number	Time (h)	Flow rate	COD (g/m³)	TNV (g/m³)	P (g/m³)	VSS (g/m³)	TSS (g/m³)
1	0	22	555	55	5	375	468.75
2	1	0	555	55	5	375	468.75
3	2	0	555	55	5	375	468.75
4	3	0	555	55	5	375	468.75
5	4	22	555	55	5	375	468.75
6	5	22	555	55	5	375	468.75
7	6	22	555	55	5	375	468.75
8	7	22	555	55	5	375	468.75
9	8	22	555	55	5	375	468.75
10	9	22	555	55	5	375	468.75
11	10	22	555	55	5	375	468.75
12	11	0	555	55	5	375	468.75
13	12	0	555	55	5	375	468.75

The flow rate at time 0 was intentionally entered as 22 m³/d to make the dynamic loading more severe for the testing of the code.

Process configuration



Process Operation

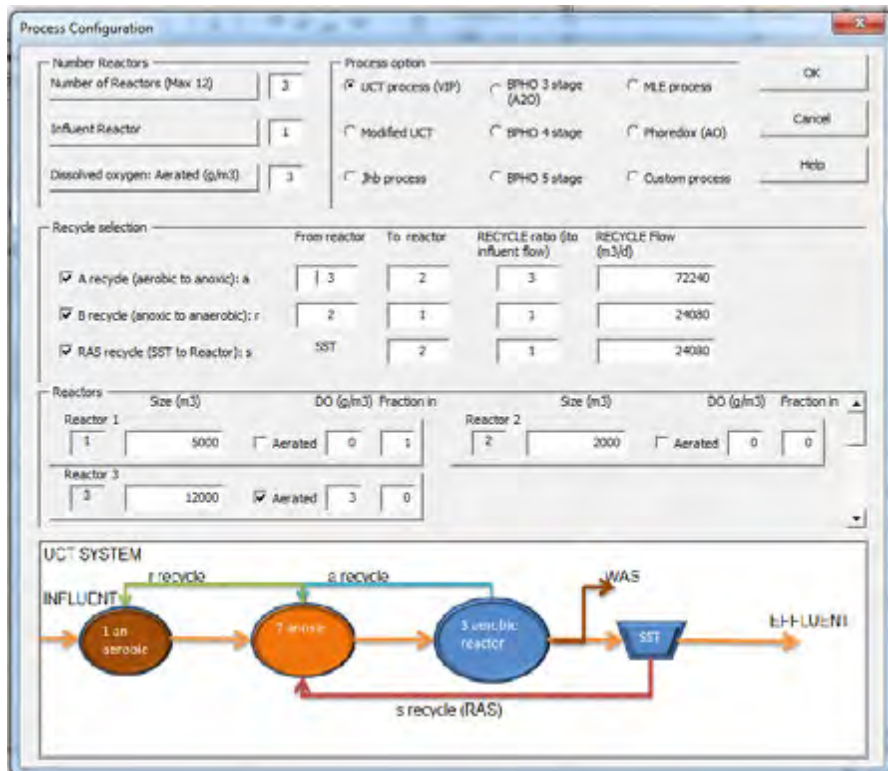


8.2. Test Data set 2 (default Kinetic and Stoichiometric constants accepted)

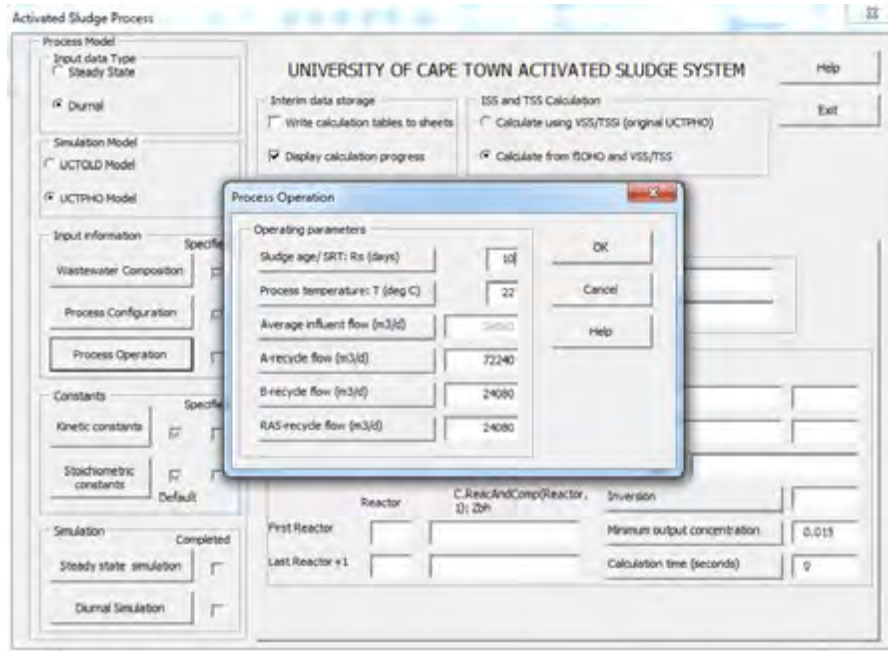
Influent wastewater (default fractions accepted)

INFLUENT WASTEWATER DATA INPUT							
Average flows and concentrations							
Flow rate (m ³ /day)	COD (g/m ³)	TKN (g/m ³)	P (g/m ³)	VSS (g/m ³)	TSS (g/m ³)		
FLOW WEIGHTED AVERAGE (g/m ³)	24080	1148.936	89.839	20.017	501.079	667.999	
Diurnal flows and concentrations							
Record number	Time (h)	Rate				Influent VSS and TSS data	
		m ³ /hour	COD (g/m ³)	TKN (g/m ³)	P (g/m ³)	VSS (g/m ³)	TSS (g/m ³)
		m ³ /day					
1	0	8640	445	37.5	8	154.7	221
2	2	11904	353	60	6	182.25	243
3	4	36288	843	87.1	14.5	496	630
4	6	41472	1165	102.1	20.9	531.2	664
5	8	34560	1304	112.6	23.1	566.4	708
6	10	28032	1334	121.6	24.1	564	752
7	12	24576	1472	102.6	26.7	630.75	841
8	14	27840	1380	93.1	23.7	557.9	797
9	16	25536	1303	84.1	21.6	511	730
10	18	23232	1227	63	19.9	495.6	708
11	20	16320	1120	60	19.1	489.4	642
12	22	10560	751	46.5	12.8	278.6	398

Process configuration



Process Operation



8.3. UCTPHO Steady State Simulations

Dataset 1: UCTPHO Steady State (VBA code) with minimum Output concentration = 0.1 mg/l

Simulation Results

STEADY STATE RESULTS: UCTPHO. ISS calc: Original TP code, Inversions = 9. Calculation time = 17 seconds

COMPOUND	UNIT	INPUT	REACTOR	1	2	3
1 Zbh (hetero.)	g COD m-3	0.0		436.5	912.2	936.0
2 Zba (auto.)	g COD m-3	0.0		14.9	29.9	30.8
3 Zbg (polyP org.)	g COD m-3	0.0		104.5	209.6	215.5
4 Ze (endog. COD)	g COD m-3	0.0		124.9	246.0	250.0
5 Zi (inert. COD)	g COD m-3	72.2		320.9	569.7	569.7
6 Sads (adsorbed COD)	g COD m-3	0.0		209.6	107.3	47.4
7 Senm (enmeshed COD)	g COD m-3	364.1		49.4	7.2	3.8
8 Sphb (PHB COD)	g COD m-3	0.0		15.4	30.6	27.6
9 Nobp (prt bio N)	g N m-3	3.6		4.8	3.3	1.9
10 Ppp (stored polyP)	g P m-3	0.0		0.0	0.1	2.1
11 ISSi (influent ISS)	g ISS m-3	150.0		667.2	1184.4	1184.4
12 Sbs.c (compl.RBCOD)	g COD m-3	81.9		15.8	0.2	0.0
13 Sbs.a (SCFA RBCOD)	g COD m-3	9.1		30.3	7.1	0.1
14 Na (ammonia N)	g N m-3	41.3		27.0	10.5	2.9
15 Nobs (sol org N)	g N m-3	3.60		1.15	1.30	1.64
16 No3 (nitrate N)	g N m-3	0.0		0.0	0.9	7.1
17 Ps (soluble P)	g P m-3	4.0		3.8	2.7	0.1
18 Sus (sol unb COD)	g COD m-3	27.8		28.3	28.7	28.9
19 Alkalinity	mole m-3	10.0		9.0	7.9	6.9
Volatile SS				862.2	1427.4	1406.0
Total SS				1149.6	1903.1	1874.6
OUR carbonaceous				0.0	0.0	21.3
OUR autotrophs				0.0	0.0	14.8
OUR total				0.0	0.0	36.1
Denit. rate				1.1	6.2	0.0
TKN				58.9	19.2	4.7

It is seen that the duration of the steady state simulation was 17 seconds.

Dataset 1: UCTPHO Steady State (Original TP version) with minimum Output concentration = 0.1 mg/l

UCTPHO

		1	2	3	
Zbh (hetero.)	=	0.0	436.5	912.2	936.1 g COD m-3
Zba (auto.)	=	0.0	14.9	29.9	30.8 g COD m-3
Zbg (polyP org.)	=	0.0	104.5	209.6	215.5 g COD m-3
Ze (endog. COD)	=	0.0	124.9	246.0	250.0 g COD m-3
Zi (inert. COD)	=	72.1	320.9	569.7	569.7 g COD m-3
Sads (adsorbed COD)	=	0.0	209.6	107.3	47.4 g COD m-3
Senm (enmeshed COD)	=	364.1	49.4	7.1	3.8 g COD m-3
Sphb (PHB COD)	=	0.0	15.4	30.6	27.6 g COD m-3
Nobp (prt bio N)	=	3.6	4.8	3.3	1.9 g N m-3
Ppp (stored polyP)	=	0.0	0.0	0.1	2.1 g P m-3
Sbs.c (compl.RBCOD)	=	81.9	15.8	0.2	0.0 g COD m-3
Sbs.a (SCFA RBCOD)	=	9.1	30.3	7.1	0.1 g COD m-3
Na (ammonia N)	=	41.3	27.0	10.5	2.9 g N m-3
Nobs (sol org N)	=	3.6	1.1	1.3	1.6 g N m-3
No3 (nitrate N)	=	0.0	0.0	0.9	7.2 g N m-3
Ps (soluble P)	=	4.0	3.8	2.7	0.1 g P m-3
Sus (sol unb COD)	=	27.7	28.3	28.7	28.9 g COD m-3
Alkalinity	=	10.0	9.0	7.9	6.9 mole m-3
Volatile SS	=		818.4	1401.8	1384.7 g USS m-3
OUR carbonaceous	=		0.0	0.0	21.2 g O2 m-3 h-1
OUR autotrophs	=		0.0	0.0	14.8 g O2 m-3 h-1
OUR total	=		0.0	0.0	36.0 g O2 m-3 h-1
Denit. rate	=		0.3	6.2	0.0 g NO3-N m-3 h-1

*** Hit any key to continue... ***

Dataset 2: UCTPHO Steady State (VBA code) with minimum Output concentration = 0.1 mg/l

Simulation Results

STEADY STATE RESULTS: UCTPHO: ISS calc: Ekama & Wentzel (2004): Inversions = 13. Calculation time = 30 seconds

COMPOUND	UNIT	INPUT	REACTOR			
			1	2	3	
1 Zbh (hetero.)	g COD m-3	0.0	1 056.6	2 219.7	2 262.7	
2 Zba (auto.)	g COD m-3	0.0	40.8	82.0	83.2	
3 Zbg (polyP org.)	g COD m-3	0.0	401.5	806.5	819.1	
4 Ze (endog. COD)	g COD m-3	0.0	624.7	1 237.0	1 249.7	
5 Zi (inert. COD)	g COD m-3	149.4	1 153.3	2 157.1	2 157.1	
6 Sads (adsorbed COD)	g COD m-3	0.0	510.5	221.7	74.0	
7 Senm (enmeshed COD)	g COD m-3	753.7	39.9	5.9	3.5	
8 Sphb (PHB. COD)	g COD m-3	0.0	87.9	53.0	28.7	
9 Nobp (prt bio N)	g N m-3	4.8	9.9	6.1	3.2	
10 Ppp (stored polyP)	g P m-3	0.0	42.3	149.4	165.2	
11 ISSi (influent ISS)	g ISS m-3	166.9	1 288.5	2 410.1	2 410.1	
12 Sbs.c (compl. RBCOD)	g COD m-3	169.6	11.9	0.1	0.1	
13 Sbs.a (SCFA RBCOD)	g COD m-3	18.8	0.3	0.1	0.1	
14 Na (ammonia N)	g N m-3	67.4	41.7	13.6	0.7	
15 Nobs (sol org N)	g N m-3	4.80	0.66	1.14	1.56	
16 No3 (nitrate N)	g N m-3	0.0	0.1	6.4	17.0	
17 Ps (soluble P)	g P m-3	17.9	51.1	17.6	0.4	
18 Sus (sol unb COD)	g COD m-3	57.4	59.8	61.5	62.2	
19 Alkalinity	mole m-3	10.0	8.3	6.0	4.4	
Volatile SS			g VSS m-3	2 645.4	4 583.0	4 512.3
Total SS			g TSS m-3	4 222.8	7 794.8	7 781.7
OUR carbonaceous			g O2 m-3 h-1	0.0	0.0	47.5
OUR autotrophs			g O2 m-3 h-1	0.0	0.0	20.1
OUR total			g O2 m-3 h-1	0.0	0.0	67.6
Denit. rate			g NO3-N m-3 h-1	13.6	14.9	0.1
TKN			g TKN m-3 h-1	44.7	16.4	3.5

It is seen that the duration of the steady state simulation was 30 seconds.

Dataset 2: UCTPHO Steady State (VBA code) with minimum Output concentration = 0.01 mg/l (Input VSS/TSSi ratio = 0.8)

Simulation Results

STEADY STATE RESULTS: UCTPHO: ISS calc: Ekama & Wentzel (2004): Inversions = 9. Calculation time = 17 seconds

COMPOUND	UNIT	INPUT	REACTOR			
			1	2	3	
1 Zbh (hetero.)	g COD m-3	0.0	1 055.8	2 219.6	2 261.5	
2 Zba (auto.)	g COD m-3	0.0	40.8	82.0	83.2	
3 Zbg (polyP org.)	g COD m-3	0.0	402.9	809.3	822.0	
4 Ze (endog. COD)	g COD m-3	0.0	624.5	1 236.6	1 249.4	
5 Zi (inert. COD)	g COD m-3	149.4	1 153.3	2 157.1	2 157.1	
6 Sads (adsorbed COD)	g COD m-3	0.0	510.6	221.7	74.0	
7 Senm (enmeshed COD)	g COD m-3	753.7	40.0	5.9	3.5	
8 Sphb (PHB. COD)	g COD m-3	0.0	88.2	53.2	28.9	
9 Nobp (prt bio N)	g N m-3	4.8	9.9	6.1	3.2	
10 Ppp (stored polyP)	g P m-3	0.0	42.2	149.3	165.2	
11 ISSi (influent ISS)	g ISS m-3	166.9	1 198.8	2 242.4	2 242.4	
12 Sbs.c (compl. RBCOD)	g COD m-3	169.6	12.0	0.1	0.0	
13 Sbs.a (SCFA RBCOD)	g COD m-3	18.8	0.3	0.0	0.0	
14 Na (ammonia N)	g N m-3	67.4	41.7	13.6	0.7	
15 Nobs (sol org N)	g N m-3	4.80	0.66	1.14	1.56	
16 No3 (nitrate N)	g N m-3	0.0	0.0	6.5	17.1	
17 Ps (soluble P)	g P m-3	17.9	51.3	17.6	0.4	
18 Sus (sol unb COD)	g COD m-3	57.4	59.8	61.5	62.2	
19 Alkalinity	mole m-3	10.0	8.3	6.0	4.4	
Volatile SS			g VSS m-3	2 646.0	4 584.1	4 513.4
Total SS			g TSS m-3	4 133.3	7 628.1	7 615.2
OUR carbonaceous			g O2 m-3 h-1	0.0	0.0	44.5
OUR autotrophs			g O2 m-3 h-1	0.0	0.0	20.1
OUR total			g O2 m-3 h-1	0.0	0.0	64.6
Denit. rate			g NO3-N m-3 h-1	2.5	14.9	0.1
TKN			g TKN m-3 h-1	44.7	16.3	3.4

Dataset 2: UCTPHO Steady State (VBA code) with minimum Output concentration = 0.001 mg/l (Input VSS/TSSi ratio = 0.8)

Display Results

SIMULATION RESULTS

Simulation Results

STEADY STATE RESULTS: UCTPHO, ISS calc: Ekama & Wentzel (2004); Inversions = 29; Calculation time = 57 seconds

COMPOUND	UNIT	INPUT	REACTOR		
			1	2	3
1 Zbh (hetero.)	g COD m-3	0.0	1 055.8	2 218.6	2 261.5
2 Zba (auto.)	g COD m-3	0.0	40.8	82.0	83.2
3 Zbg (polyP org.)	g COD m-3	0.0	402.9	809.3	822.0
4 Ze (endog. COD)	g COD m-3	0.0	624.5	1 236.6	1 249.4
5 Zi (inert. COD)	g COD m-3	149.4	1 153.3	2 157.1	2 157.1
6 Sads (adsorbed COD)	g COD m-3	0.0	510.6	221.7	74.0
7 Sann (enmeshed COD)	g COD m-3	753.7	40.0	5.9	3.5
8 Sphb (PHB COD)	g COD m-3	0.0	88.2	53.2	28.9
9 Nobp (prt bio N)	g N m-3	4.8	9.9	6.1	3.2
10 Ppp (stored polyP)	g P m-3	0.0	42.2	149.3	165.2
11 ISSi (influent ISS)	g ISS m-3	194.1	1 498.5	2 802.9	2 802.9
12 Sbs,c (compl RBCOD)	g COD m-3	169.6	12.0	0.1	0.0
13 Sbs,a (SCFA RBCOD)	g COD m-3	18.8	0.3	0.0	0.0
14 Na (ammonia N)	g N m-3	67.4	41.7	13.6	0.7
15 Nobs (sol org N)	g N m-3	4.80	0.66	1.14	1.56
16 No3 (nitrate N)	g N m-3	0.0	0.0	6.5	17.1
17 Ps (soluble P)	g P m-3	17.9	51.3	17.6	0.4
18 Sus (sol unb COD)	g COD m-3	57.4	59.8	61.5	62.2
19 Alkalinity	mole m-3	10.0	8.3	6.0	4.4
Volatile SS			2 646.0	4 584.1	4 513.4
Total SS			4 433.0	8 188.7	8 175.8
OUR carbonaceous			0.0	0.0	44.2
OUR autotrophs			0.0	0.0	20.1
OUR total			0.0	0.0	64.3
Denit. rate			1.3	14.9	0.1
TKN			44.7	16.3	3.4

Dataset 2: UCTPHO Steady State (Original TP version) with minimum Output concentration = 0.1 mg/l

UCTPHO

		1	2	3	
Zbh (hetero.)	=	0.0	1056.3	2219.3	2262.3 g COD m-3
Zba (auto.)	=	0.0	40.9	82.1	83.4 g COD m-3
Zbg (polyP org.)	=	0.0	402.0	807.5	820.1 g COD m-3
Ze (endog. COD)	=	0.0	624.6	1236.9	1249.6 g COD m-3
Zi (inert. COD)	=	149.4	1153.3	2157.1	2157.1 g COD m-3
Sads (adsorbed COD)	=	0.0	510.5	221.7	74.0 g COD m-3
Sann (enmeshed COD)	=	753.7	40.0	5.9	3.5 g COD m-3
Sphb (PHB COD)	=	0.0	88.0	53.1	28.8 g COD m-3
Nobp (prt bio N)	=	4.8	9.9	6.1	3.2 g N m-3
Ppp (stored polyP)	=	0.0	42.3	149.3	165.2 g P m-3
Sbs,c (compl RBCOD)	=	169.6	11.9	0.1	0.0 g COD m-3
Sbs,a (SCFA RBCOD)	=	18.8	0.3	0.0	0.0 g COD m-3
Na (ammonia N)	=	67.5	41.7	13.6	0.7 g N m-3
Nobs (sol org N)	=	4.8	0.7	1.1	1.6 g N m-3
No3 (nitrate N)	=	0.0	0.0	6.5	17.2 g N m-3
Ps (soluble P)	=	17.9	51.2	17.6	0.4 g P m-3
Sus (sol unb COD)	=	57.4	59.8	61.5	62.2 g COD m-3
Alkalinity	=	10.0	8.3	6.0	4.4 mole m-3
Volatile SS	=		2559.2	4543.7	4490.9 g VSS m-3
OUR carbonaceous	=		0.0	0.0	44.2 g O2 m-3 h-1
OUR autotrophs	=		0.0	0.0	20.2 g O2 m-3 h-1
OUR total	=		0.0	0.0	64.4 g O2 m-3 h-1
Denit. rate	=		1.3	14.9	0.1 g NO3-N m-3 h-1

*** Hit any key to continue ***

8.4. UCTPHO Diurnal Simulations

Dataset 1: UCTPHO Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

No	COMPOUND	UNIT	INPUT	REACTOR		
				1	2	3
1	Zbh (hetero.)	g COD m-3	653.2	865.8	915.1	
2	Zba (auto.)	g COD m-3	21.1	26.5	28.0	
3	Zbg (polyP org.)	g COD m-3	142.5	178.7	188.0	
4	Zf (endog COD)	g COD m-3	181.8	223.3	232.6	
5	Zi (inert COD)	g COD m-3	437.2	519.5	537.7	
6	Sads (adsorbed COD)	g COD m-3	218.8	83.9	50.5	
7	Serm (enmeshed COD)	g COD m-3	5.2	3.8	3.6	
8	Sphb (PHB COD)	g COD m-3	22.0	26.2	25.0	
9	Nobp (prt bio N)	g N m-3	6.7	3.4	2.4	
10	Ppp (stored polyP)	g P m-3	0.0	0.0	0.8	
11	iSSi (influent iSS)	g iSS m-3	75.0	89.1	92.3	
12	Sbs.c (compl RBCOD)	g COD m-3	0.0	0.0	0.0	
13	Sbs.a (SCFA RBCOD)	g COD m-3	22.0	3.9	0.1	
14	Na (ammonia N)	g N m-3	18.6	6.2	1.7	
15	Nobs (sol org N)	g N m-3	0.5	1.5	1.9	
16	No3 (nitrate N)	g N m-3	0.0	3.3	9.2	
17	Ps (soluble P)	g P m-3	2.94	1.22	0.02	
18	Sus (sol unb COD)	g COD m-3	28.5	28.7	28.7	
19	Alkalinity	mole m-3	8.5	7.4	6.7	
23	Volatile solids	g VSS m-3	1136.4	1302.5	1338.1	
25	Total solids	g TSS m-3	1515.1	1736.7	1784.2	
20	OUR carb	g O2 m-3 h-1	0.0	0.0	19.9	
21	OUR nitr	g O2 m-3 h-1	0.0	0.0	10.8	
22	OUR tot	g O2 m-3 h-1	0.0	0.0	30.7	
26	Denitrification rate	g NO3-N m-3 h-1				
24	TKN	g N m-3	20.8	9.3	5.3	

The calculation time of this diurnal simulation was 25.45 minutes.

Dataset 1: UCTPHO Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

***** DIURNAL RESPONSE RESULTS ***** UCTPHO										
Reactor 3 Cycle number 5										
TIME	Zbh	Zba	Zbg	Sads	Sphb	Ppp	Sbsc	No3	Ps	Ot
0.0	914.2	28.2	189.8	50.4	24.8	0.9	0.0	9.2	0.0	30.6
2.0	958.0	29.5	199.5	58.5	26.4	1.0	0.0	7.2	0.1	37.6
4.0	938.0	28.9	194.8	34.4	24.2	0.9	0.0	7.9	0.0	29.5
6.0	904.3	28.2	190.0	18.8	21.6	0.9	0.0	7.7	0.0	22.1
8.0	875.1	27.8	187.6	13.8	19.2	1.1	0.0	7.1	0.0	18.1
10.0	924.2	29.7	201.0	34.4	20.5	1.3	0.0	5.5	0.1	32.0
12.0	942.1	30.3	205.2	63.3	22.6	1.4	0.0	5.7	0.3	39.5
14.0	945.5	30.3	205.1	88.5	24.7	1.5	0.0	6.2	0.3	42.4
16.0	947.8	30.1	204.1	109.0	26.5	1.5	0.0	6.6	0.3	43.7
18.0	951.1	29.9	202.8	125.9	28.2	1.6	0.0	6.7	0.3	44.5
20.0	955.4	29.7	201.6	140.2	29.7	1.6	0.0	6.8	0.2	45.0
22.0	935.8	28.8	194.1	95.2	27.3	1.2	0.0	8.7	0.0	38.9
24.0	915.1	28.0	188.0	50.4	25.0	0.8	0.0	9.2	0.0	30.8

Dataset 1: UCTPHO Diurnal Simulation (TP code) with Accuracy% = 0.5 and Theta = 0.7

***** DIURNAL RESPONSE RESULTS *****

Reactor 3 Cycle number 7

TIME	Zbh	Zba	Zbg	Sads	Sphb	Ppp	Sbsc	No3	Ps	Ot
0.0	913.6	27.9	186.7	50.7	24.8	1.1	0.0	9.2	0.0	31.0
2.0	957.5	29.3	196.3	58.7	26.4	1.2	0.0	7.2	0.1	37.5
4.0	937.5	28.7	191.7	34.6	24.2	1.1	0.0	7.9	0.0	29.7
6.0	903.9	27.9	186.9	18.9	21.7	1.1	0.0	7.7	0.0	22.3
8.0	874.9	27.5	184.7	13.8	19.2	1.3	0.0	7.2	0.0	18.2
10.0	924.0	29.4	197.9	34.2	20.5	1.6	0.0	5.5	0.1	31.9
12.0	941.7	30.1	202.1	63.1	22.6	1.7	0.0	5.7	0.3	39.3
14.0	944.8	30.0	202.1	88.5	24.7	1.7	0.0	6.2	0.3	42.3
16.0	946.8	29.9	201.1	109.2	26.5	1.8	0.0	6.5	0.3	43.6
18.0	949.8	29.7	199.9	126.4	28.1	1.8	0.0	6.7	0.3	44.4
20.0	953.8	29.4	198.8	140.9	29.7	1.8	0.0	6.8	0.2	44.9
22.0	934.3	28.6	191.4	95.9	27.3	1.5	0.0	8.6	0.0	38.9
24.0	913.9	27.8	185.4	50.7	24.9	1.1	0.0	9.2	0.0	31.1

Integration time = 0.10

Dataset 2: UCTPHO Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

Display Results

SIMULATION RESULTS

Simulation Results

DIURNAL RESULTS: UCTPHO; ISS calc: Ekama & Wentzel (2004); Cycles = 2; Runtime = 18.583 minutes and *** Dynamic solution reached***

No	COMPOUND	UNIT	REACTOR		
			INPUT	1	2
1	Zbh (hetero.)	g COD m-3	1277.3	2152.3	2246.6
2	Zba (auto.)	g COD m-3	48.9	78.3	81.2
3	Zbg (polyP org.)	g COD m-3	476.7	766.5	796.7
4	Ze (endog COD)	g COD m-3	740.9	1172.7	1212.7
5	Zi (inert COD)	g COD m-3	1336.9	2044.1	2100.1
6	Sads (adsorbed COD)	g COD m-3	464.1	153.9	52.4
7	Senm (anmeshed COD)	g COD m-3	12.2	4.4	3.4
8	Sphb (PHB COD)	g COD m-3	75.0	45.1	29.9
9	Nobp (prt bio N)	g N m-3	10.2	5.0	2.6
10	Ppp (stored polyP)	g P m-3	63.8	141.7	156.1
11	ISSi (influent ISS)	g ISS m-3	1497.4	2281.9	2343.5
12	Sbs.c (compl RBCOD)	g COD m-3	1.9	0.0	0.0
13	Sbs.a (SCFA RBCOD)	g COD m-3	0.0	0.0	0.0
14	Na (ammonia N)	g N m-3	23.9	6.3	0.3
15	Nobs (sol org N)	g N m-3	0.3	1.1	1.5
16	No3 (nitrate N)	g N m-3	0.0	5.9	14.0
17	Ps (soluble P)	g P m-3	40.20	11.53	0.09
18	Sus (sol unb COD)	g COD m-3	60.4	64.2	65.3
19	Alkalinity	mole m-3	7.6	5.7	4.6
23	Volatile solids	g VSS m-3	2994.7	4336.9	4407.5
25	Total solids	g TSS m-3	4862.0	7363.1	7576.2
20	OUR carb	g O2 m-3 h-1	0.0	0.0	37.3
21	OUR nitr	g O2 m-3 h-1	0.0	0.0	10.3
22	OUR tot	g O2 m-3 h-1	0.0	0.0	47.5
26	Denitrification rate	g NO3-N m-3 h-1			
24	TKN	g N m-3	25.6	8.9	3.3

It is seen that the duration of the diurnal simulation was 18.58 minutes.

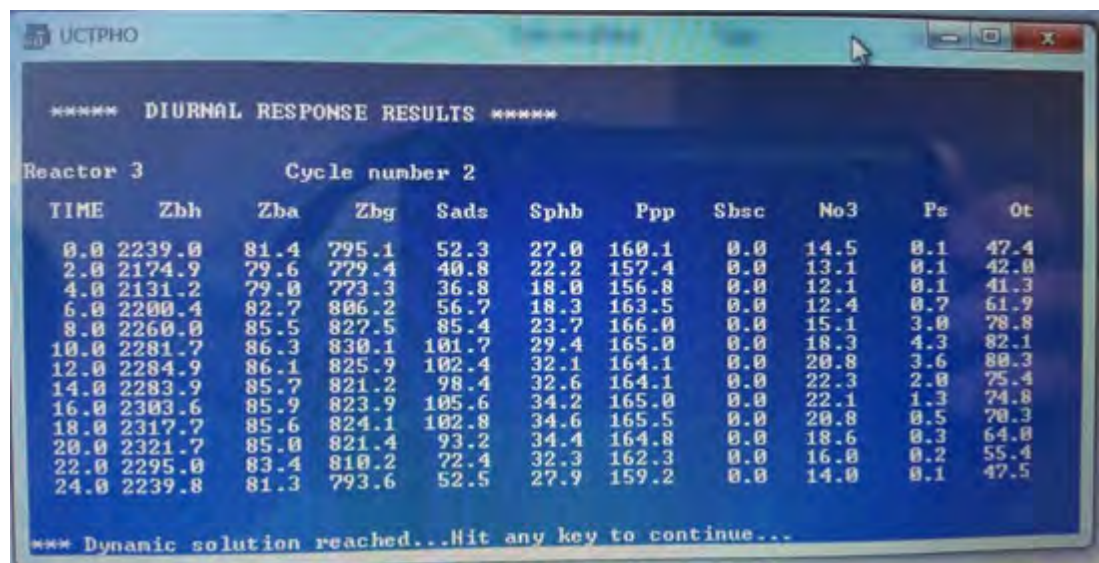
Dataset 2: UCTPHO Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

***** DIURNAL RESPONSE RESULTS ***** UCTPHO										
Reactor 3 Cycle number 2										
TIME	Zbh	Zba	Zbg	Sads	Sphb	Ppp	Sbsc	No3	Ps	Ot
0.0	2 238.5	81.2	798.0	52.4	27.0	159.5	0.0	14.5	0.1	47.4
2.0	2 174.3	79.5	782.2	40.9	21.8	157.0	0.0	13.0	0.1	42.0
4.0	2 130.6	78.8	776.0	36.9	17.7	156.5	0.0	12.0	0.1	41.4
6.0	2 199.8	82.5	808.9	56.8	18.1	163.1	0.0	12.3	0.8	61.9
8.0	2 259.5	85.4	830.3	85.5	23.6	165.6	0.0	15.1	3.1	78.8
10.0	2 281.2	86.2	832.9	101.7	29.3	164.5	0.0	18.3	4.4	82.0
12.0	2 284.5	85.9	828.6	102.5	32.0	163.6	0.0	20.7	3.7	80.2
14.0	2 283.5	85.5	823.8	98.5	32.6	163.6	0.0	22.2	2.0	75.3
16.0	2 303.2	85.7	826.5	105.6	34.2	164.5	0.0	22.0	1.3	74.8
18.0	2 317.4	85.4	826.7	102.9	34.6	165.0	0.0	20.7	0.5	70.3
20.0	2 321.3	84.8	823.9	93.3	34.4	164.3	0.0	18.6	0.3	64.0
22.0	2 294.7	83.2	812.8	72.5	32.3	161.9	0.0	16.0	0.2	55.5
24.0	2 239.4	81.2	796.1	52.5	27.7	158.9	0.0	14.0	0.1	47.5

Dataset 2: UCTPHO Diurnal Simulation (VBA code) with Accuracy% = 0.5 and Theta = 0.7

***** DIURNAL RESPONSE RESULTS ***** UCTPHO										
Reactor 3 Cycle number 2										
TIME	Zbh	Zba	Zbg	Sads	Sphb	Ppp	Sbsc	No3	Ps	Ot
0.0	2 241.9	81.2	795.6	52.3	28.5	158.6	0.0	14.4	0.1	47.4
2.0	2 177.6	79.5	780.1	40.9	24.4	155.3	0.0	13.0	0.1	42.0
4.0	2 133.9	78.8	774.2	37.0	20.7	154.2	0.0	12.0	0.1	41.4
6.0	2 203.4	82.5	807.6	56.8	20.3	161.2	0.0	12.3	0.5	62.0
8.0	2 263.4	85.4	829.3	85.3	25.0	164.2	0.0	15.0	2.5	78.9
10.0	2 285.3	86.1	832.3	101.5	30.2	163.4	0.0	18.2	3.6	82.1
12.0	2 288.7	85.9	828.2	102.3	32.7	162.7	0.0	20.7	2.8	80.2
14.0	2 287.8	85.5	823.5	98.3	33.2	162.7	0.0	22.1	1.3	75.3
16.0	2 307.7	85.7	826.2	105.3	34.9	163.5	0.0	22.0	0.9	74.8
18.0	2 322.0	85.4	826.3	102.7	35.5	163.7	0.0	20.7	0.4	70.3
20.0	2 326.1	84.8	823.6	92.9	35.2	162.9	0.0	18.5	0.3	64.0
22.0	2 299.5	83.2	812.5	72.2	33.0	160.5	0.0	16.0	0.1	55.5
24.0	2 244.2	81.2	795.9	52.4	29.5	156.8	0.0	13.9	0.1	47.5

Dataset 2: UCTPHO Diurnal Simulation (TP code) with Accuracy% = 0.5 and Theta = 0.7



Data set 2: UCTOLD Steady State Simulation (VBA code) with minimum Output concentration = 0.1 mg/l

SIMULATION RESULTS						
STEADY STATE RESULTS: UCTOLD; ISS calc: Ekama & Wentzel (2004); Inversions = 8; Calculation time = 15 seconds						
	COMPOUND	UNIT	INPUT	REACTOR		
				1	2	3
1	Zbh (hetero.)	g COD m-3	0.0	1 199.5	2 542.8	2 592.2
2	Zba (auto.)	g COD m-3	0.0	42.4	85.1	86.5
3	Zbg (polyP org.)	g COD m-3	0.0	0.1	0.1	0.1
4	Ze (endog. COD)	g COD m-3	0.0	665.7	1 318.2	1 331.8
5	Zi (inert. COD)	g COD m-3	149.4	1 153.3	2 157.1	2 157.1
6	Sads (adsorbed COD)	g COD m-3	0.0	546.0	254.4	84.2
7	Senm (enmeshed COD)	g COD m-3	753.7	34.4	5.3	3.5
8	Sphb (PHB COD)	g COD m-3	0.0	0.1	0.1	0.1
9	Nobp (pt bio N)	g N m-3	4.8	12.2	9.4	5.6
10	Ppp (stored polyP)	g P m-3	0.0	0.1	0.1	0.1
11	ISSi (influent ISS)	g ISS m-3	166.9	1 288.5	2 410.1	2 410.1
12	Sbs.c (compt. RBCOD)	g COD m-3	188.4	81.3	0.6	0.1
13	Sbs.a (SCFA RBCOD)	g COD m-3	0.0	0.1	0.1	0.1
14	Na (ammonia N)	g N m-3	67.4	41.8	13.0	0.7
15	Nobs (sol org N)	g N m-3	4.80	0.55	0.87	1.57
16	No3 (nitrate N)	g N m-3	0.0	0.1	3.2	14.3
17	Ps (soluble P)	g P m-3	17.9	17.9	17.9	17.9
18	Sus (sol unb COD)	g COD m-3	57.4	57.4	57.4	57.4
19	Alkalinity	mole m-3	10.0	8.2	5.9	4.2
	Volatile SS	g VSS m-3		2 460.5	4 299.4	4 226.8
	Total SS	g TSS m-3		3 873.5	6 972.7	6 905.1
	OUR carbonaceous	g O2 m-3 h-1		0.0	0.0	50.7
	OUR autotrophs	g O2 m-3 h-1		0.0	0.0	20.9
	OUR total	g O2 m-3 h-1		0.0	0.0	71.6
	Denit. rate	g NO3-N m-3 h-1		21.4	18.9	0.1
	TKN	g TKN m-3 h-1		44.6	15.8	3.5

It is seen that the duration of the steady state simulation was 15 seconds.

Data set 2: UCTOLD Steady State Simulation (TP code) with minimum Output concentration = 0.1 mg/l

COMPOUND	INPUT	REACTOR			
		1	2	3	
Zbh (hetero.)	0.0	1205.5	2537.3	2590.4	g COD m-3
Zba (autotrophs)	0.0	42.6	85.6	86.9	g COD m-3
Ze (endog.)	0.0	665.7	1318.2	1331.7	g COD m-3
Zi (prt unb COD)	149.4	1153.3	2157.1	2157.1	g COD m-3
Sads (adsorb. COD)	0.0	549.7	263.5	87.9	g COD m-3
Senm (enmesh COD)	753.7	34.3	5.3	3.5	g COD m-3
Nobp (prt bio N)	4.8	12.4	9.7	5.7	g N m-3
Sbs (sol bio COD)	188.4	68.9	0.5	0.0	g COD m-3
Na (ammonia N)	67.5	41.4	13.2	0.7	g N m-3
Nobs (sol org N)	4.8	0.5	0.8	1.6	g N m-3
NO3 (nitrate N)	0.0	0.0	6.6	17.8	g N m-3
Alkalinity	10.0	0.1	5.7	4.0	mole m-3
Sus (sol unb COD)	57.4	57.4	57.4	57.4	g COD m-3
Volatile SS		2467.0	4302.0	4228.1	g VSS m-3
Total SS		3289.3	5736.0	5637.5	g TSS m-3
OUR heterotrophs		0.0	0.0	46.7	g O2 m-3 h-1
OUR autotrophs		0.0	0.0	21.0	g O2 m-3 h-1
OUR total		0.0	0.0	67.7	g O2 m-3 h-1
Denit. rate		1.3	15.7	0.1	g NO3-N m-3 h-1
TKN		44.6	16.7	4.9	g N m-3

*** Hit any key to continue...

8.6. UCTOLD Diurnal simulations

Data set 1: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

No	COMPOUND	UNIT	INPUT	REACTOR		
				1	2	3
1	Zbh (hetero.)	g COD m-3		728.6	964.6	1022.4
2	Zba (auto.)	g COD m-3		22.0	27.7	29.2
3	Zbg (polyP org.)	g COD m-3		0.1	0.1	0.1
4	Ze (endog. COD)	g COD m-3		196.1	240.9	250.8
5	Zi (inert. COD)	g COD m-3		438.1	520.7	539.0
6	Sads (adsorbed COD)	g COD m-3		247.0	99.6	56.5
7	Senm (enmeshed COD)	g COD m-3		5.1	3.6	3.6
8	Sphb (PHB COD)	g COD m-3		0.1	0.1	0.1
9	Nobp (prt bio N)	g N m-3		9.4	6.0	4.5
10	Ppp (stored polyP)	g P m-3		0.1	0.1	0.1
11	ISSi (influent ISS)	g ISS m-3	1107.5	1316.2	1362.4	
12	Sbs.c (compl.RBCOD)	g COD m-3		9.9	0.0	0.0
13	Sbs.a (SCFA.RBCOD)	g COD m-3		0.0	0.0	0.0
14	Na (ammonia N)	g N m-3		17.6	5.2	1.1
15	Nobs (sol org N)	g N m-3		0.3	1.4	2.1
16	NO3 (nitrate N)	g N m-3		0.0	3.0	8.7
17	Ps (soluble P)	g P m-3		3.99	3.99	3.99
18	Sus (sol unb COD)	g COD m-3		27.8	27.8	27.8
19	Alkalinity	mole m-3		8.3	7.2	6.5
23	Volatle solids	g VSS m-3		1106.1	1255.0	1284.8
25	Total solids	g TSS m-3		2288.9	2670.6	2752.7
20	OUR carb	g O2 m-3 h-1		0.0	0.0	21.7
21	OUR nitr	g O2 m-3 h-1		0.0	0.0	9.5
22	OUR tot	g O2 m-3 h-1		0.0	0.0	31.2
26	Denitrification rate	g NO3-N m-3 h-1				
24	TKN	g N m-3		19.6	8.3	4.0

It is seen that the duration of the diurnal simulation was 6.37 minutes.

Data set 1: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 0.5 and Theta = 0.7

DIURNAL RESULTS: UCTOLD: ISS calc: Ekama & Wentzel (2004). Cycles = 3: Runtime = 14.133 minutes and *** Dynamic solution reached***

No	COMPOUND	UNIT	INPUT	REACTOR		
				1	2	3
1	Zbh (hetero.)	g COD m-3		723.9	961.6	1019.7
2	Zba (auto.)	g COD m-3		21.6	27.2	28.7
3	Zbg (polyP org.)	g COD m-3		0.0	0.0	0.0
4	Ze (endog. COD)	g COD m-3		195.1	239.7	249.6
5	Zi (inert. COD)	g COD m-3		437.2	519.5	537.7
6	Sads (adsorbed COD)	g COD m-3		248.5	100.9	57.5
7	Senm (enmeshed COD)	g COD m-3		5.2	3.8	3.6
8	Sphb (PHB COD)	g COD m-3		0.0	0.0	0.0
9	Nobp (prt bio N)	g N m-3		9.4	6.1	4.5
10	Ppp (stored polyP)	g P m-3		0.0	0.0	0.0
11	ISSi (influent ISS)	g ISS m-3		1 105.1	1 313.1	1 359.3
12	Sbs.c (compl RBCOD)	g COD m-3		10.1	0.1	0.0
13	Sbs.a (SCFA RBCOD)	g COD m-3		0.0	0.0	0.0
14	Na (ammonia N)	g N m-3		17.7	5.4	1.2
15	Nobs (sol org N)	g N m-3		0.3	1.4	2.1
16	No3 (nitrate N)	g N m-3		0.0	3.0	8.8
17	Ps (soluble P)	g P m-3		3.99	3.99	3.99
18	Sus (sol unb COD)	g COD m-3		27.8	27.8	27.8
19	Alkalinity	mole m-3		8.3	7.2	6.5
23	Volatile solids	g VSS m-3		1 102.4	1 251.8	1 281.7
25	Total solids	g TSS m-3		2 282.2	2 664.0	2 745.9
20	OUR carb	g O2 m-3 h-1		0.0	0.0	21.8
21	OUR nitr	g O2 m-3 h-1		0.0	0.0	9.9
22	OUR tot	g O2 m-3 h-1		0.0	0.0	31.7
26	Denitrification rate	g NO3-N m-3 h-1				
24	TKN	g N m-3		19.7	8.5	5.0

It is seen that the duration of the diurnal simulation was 14.1 minutes.

Data set 1: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

***** DIURNAL RESPONSE RESULTS ***** UCTOLD										
Reactor 3 Cycle number 2										
TIME	Zbh	Zba	Sads	Senm	VSS	Sbsc	Na	No3	TKN	Ot
0.0	1 019.3	29.4	56.6	3.6	1 283.8	0.0	1.0	8.7	4.8	31.0
2.0	1 067.6	30.8	67.1	4.0	1 353.7	0.0	3.1	6.7	6.6	38.9
4.0	1 046.0	30.2	39.4	3.5	1 305.4	0.0	1.6	7.5	5.2	31.4
6.0	1 010.1	29.4	20.9	3.4	1 253.0	0.0	1.1	7.4	4.7	24.1
8.0	978.8	29.1	14.5	3.5	1 219.9	0.0	0.9	7.0	4.2	19.9
10.0	1 032.8	31.1	38.5	3.9	1 314.5	0.0	2.3	5.4	5.4	33.4
12.0	1 052.2	31.7	71.1	4.2	1 364.5	0.0	4.0	5.8	7.1	40.8
14.0	1 055.9	31.7	98.9	4.7	1 387.5	0.0	5.2	6.3	8.3	43.7
16.0	1 058.0	31.5	122.1	4.7	1 402.7	0.0	6.1	6.6	9.2	45.0
18.0	1 061.2	31.3	140.8	5.2	1 415.2	0.0	6.7	6.8	9.8	45.8
20.0	1 065.4	31.0	157.5	4.9	1 426.4	0.0	7.1	6.8	10.2	46.3
22.0	1 044.1	30.1	106.9	3.8	1 353.1	0.0	3.1	8.7	6.5	40.4
24.0	1 022.4	29.2	56.5	3.6	1 284.8	0.0	1.1	8.7	4.8	31.2

Data set 1: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 0.5 and Theta = 0.7

***** DIURNAL RESPONSE RESULTS ***** UCTOLD *** Dynamic solution reached***										
Reactor 3 Cycle number 3										
TIME	Zbh	Zba	Sads	Senm	VSS	Sbsc	Na	No3	TKN	Ot
0.0	1 020.4	28.8	57.3	3.6	1 282.5	0.0	1.2	8.8	4.9	31.6
2.0	1 068.3	30.2	67.7	4.0	1 352.1	0.0	3.2	6.7	6.7	38.8
4.0	1 046.7	29.6	39.8	3.5	1 303.6	0.0	1.7	7.5	5.4	31.6
6.0	1 010.5	28.9	21.0	3.4	1 251.0	0.0	1.2	7.5	4.7	24.3
8.0	978.9	28.5	14.6	3.4	1 217.7	0.0	0.9	7.1	4.2	20.0
10.0	1 032.4	30.5	38.5	3.8	1 311.7	0.0	2.3	5.5	5.5	33.2
12.0	1 051.2	31.2	71.2	4.2	1 361.5	0.0	4.1	5.7	7.2	40.6
14.0	1 054.5	31.1	99.5	4.4	1 384.4	0.0	5.4	6.2	8.5	43.5
16.0	1 056.2	30.9	122.8	4.6	1 399.5	0.0	6.3	6.5	9.4	44.8
18.0	1 058.9	30.7	142.3	4.7	1 412.0	0.0	6.9	6.7	10.0	45.6
20.0	1 062.8	30.5	158.9	4.8	1 423.2	0.0	7.4	6.7	10.5	46.1
22.0	1 041.4	29.5	108.3	3.8	1 350.1	0.0	3.3	8.6	6.7	40.5
24.0	1 019.7	28.7	57.5	3.6	1 281.7	0.0	1.2	8.8	5.0	31.7

Data set 1: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 0.1 and Theta = 0.7 (after 43.5 minutes and 16 cycles)

***** DIURNAL RESPONSE RESULTS ***** UCTOLD										
Reactor 3 Cycle number 16										
TIME	Zbh	Zba	Sads	Senm	VSS	Sbsc	Na	No3	TKN	Ot
0.0	989.8	27.3	137.2	3.9	1 309.4	0.0	1.6	19.9	5.1	36.1
2.0	1 032.1	28.6	158.6	4.6	1 382.2	0.0	3.3	18.9	6.7	41.3
4.0	1 014.8	28.0	123.9	3.9	1 332.2	0.0	1.6	20.5	5.2	36.3
6.0	990.1	27.3	87.6	3.7	1 275.5	0.0	0.8	21.7	4.6	31.1
8.0	972.3	26.9	60.4	3.6	1 237.4	0.0	0.7	22.7	4.7	28.2
10.0	1 024.2	28.8	89.8	4.1	1 333.7	0.0	2.6	21.9	6.2	37.9
12.0	1 042.8	29.4	123.6	4.5	1 383.9	0.0	4.8	20.0	8.2	42.4
14.0	1 044.5	29.4	153.5	4.8	1 407.1	0.0	6.5	18.1	9.7	44.3
16.0	1 043.3	29.3	180.3	5.0	1 422.8	0.0	7.6	16.6	10.7	45.1
18.0	1 042.1	29.1	204.7	5.3	1 436.2	0.0	8.3	15.4	11.4	45.6
20.0	1 041.6	28.9	227.2	5.5	1 448.6	0.0	8.7	14.5	11.8	45.8
22.0	1 014.9	28.0	183.4	4.2	1 376.7	0.0	4.7	17.4	7.9	42.3
24.0	989.8	27.3	137.2	3.9	1 309.4	0.0	1.6	19.9	5.1	36.1

Data set 1: UCTOLD Diurnal Simulation (TP code) with Accuracy% = 0.5 and Theta = 0.7

***** DIURNAL RESPONSE RESULTS *****

Reactor 3 Cycle number 6

TIME	Zbh	Zba	Sads	Senn	USS	Sbs	Na	No3	TKN	Ot
0.0	1015.3	28.7	63.3	3.6	1282.2	0.0	1.3	10.4	4.9	32.4
2.0	1060.4	30.1	78.2	4.1	1352.7	0.0	3.2	8.9	6.7	39.4
4.0	1039.2	29.5	49.8	3.6	1304.3	0.0	1.7	10.1	5.3	32.9
6.0	1004.6	28.7	28.9	3.5	1251.4	0.0	1.1	10.7	4.7	26.2
8.0	975.0	28.4	19.7	3.5	1217.5	0.0	0.9	10.9	4.3	21.9
10.0	1029.1	30.4	42.8	3.9	1311.3	0.0	2.3	9.1	5.6	33.8
12.0	1051.5	31.0	70.2	4.2	1359.9	0.0	4.1	7.9	7.3	40.2
14.0	1057.1	31.0	94.8	4.4	1381.9	0.0	5.5	7.2	8.6	43.0
16.0	1059.5	30.8	117.0	4.6	1396.8	0.0	6.5	7.0	9.6	44.5
18.0	1062.0	30.6	136.8	4.8	1409.4	0.0	7.1	6.9	10.2	45.3
20.0	1065.2	30.3	154.3	4.9	1420.8	0.0	7.6	6.9	10.7	45.9
22.0	1040.8	29.4	100.3	3.8	1348.8	0.0	3.6	9.3	7.0	40.7
24.0	1015.3	28.6	63.4	3.6	1281.9	0.0	1.3	10.4	5.0	32.5

*** Dynamic solution reached...Hit any key to continue...*

Data set 2: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

Display Results

SIMULATION RESULTS

Simulation Results

DIURNAL RESULTS: UCTOLD: ISS calc: Ekama & Wentzel (2004): Cycles = 2; Runtime = 17.65 minutes and *** Dynamic solution reached***

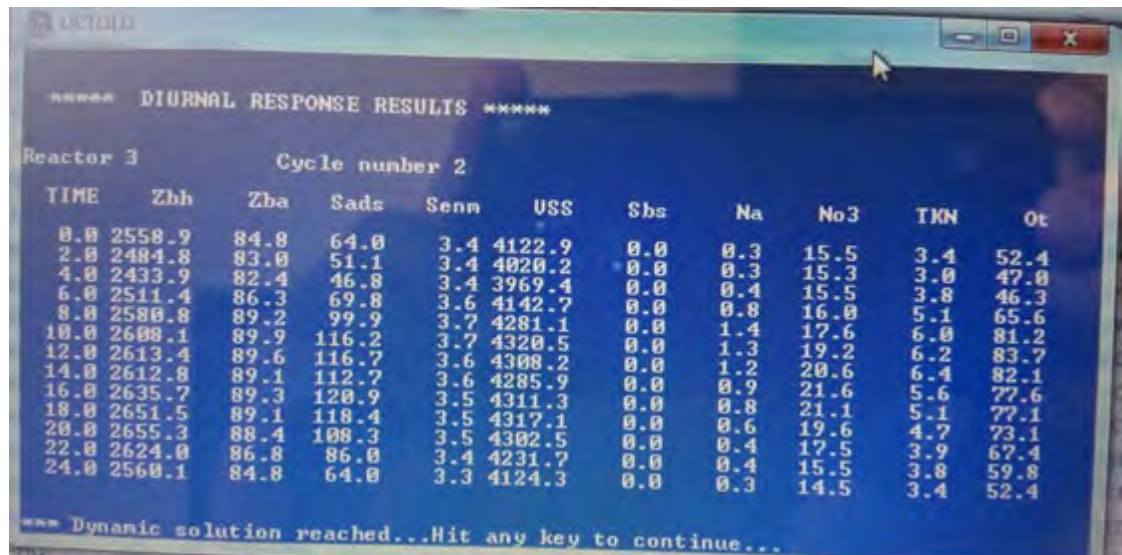
No	COMPOUND	UNIT	INPUT	REACTOR	1	2	3
1	Zbh (hetero.)	g COD m-3			1455.5	2466.7	2579.0
2	Zba (auto.)	g COD m-3			50.8	81.3	84.4
3	Zbg (polyP org.)	g COD m-3			0.1	0.1	0.1
4	Zc (endog. COD)	g COD m-3			789.7	1 250.1	1 292.8
5	Zi (inert. COD)	g COD m-3			1 336.9	2 044.0	2 100.1
6	Sads (adsorbed COD)	g COD m-3			507.2	103.8	60.7
7	Senn (enmeshed COD)	g COD m-3			11.0	4.3	3.3
8	Sphb (PHB COD)	g COD m-3			0.1	0.1	0.1
9	Nobp (pt bio N)	g N m-3			13.3	8.0	4.7
10	Ppp (stored polyP)	g P m-3			0.1	0.1	0.1
11	ISSi (influent ISS)	g ISS m-3			1 497.4	2 281.9	2 343.5
12	Sbs,c (compl RBCOD)	g COD m-3			51.1	0.3	0.0
13	Sbs,a (SCFA RBCOD)	g COD m-3			0.0	0.0	0.0
14	Na (ammonia N)	g N m-3			24.1	6.1	0.3
15	Nobs (sol org N)	g N m-3			0.2	0.9	1.6
16	No3 (nitrate N)	g N m-3			0.0	3.4	11.4
17	Pa (soluble P)	g P m-3			17.64	18.55	18.80
18	Sus (sol unb COD)	g COD m-3			57.5	59.9	60.5
19	Alkalinity	mole m-3			7.5	5.5	4.4
23	Volatile acids	g VSS m-3			2 805.0	4 074.7	4 135.5
25	Total solids	g TSS m-3			4 453.2	6 611.7	6 745.6
20	OUR carb	g O2 m-3 h-1			0.0	0.0	39.5
21	OUR nitr	g O2 m-3 h-1			0.0	0.0	12.2
22	OUR tot	g O2 m-3 h-1			0.0	0.0	51.7
26	Denitrification rate	g NO3-N m-3 h-1					
24	TKN	g N m-3			25.8	8.5	3.4

It is seen that the duration of the diurnal simulation was 17.65 minutes.

Data set 2: UCTOLD Diurnal Simulation (VBA code) with Accuracy% = 1.0 and Theta = 0.5

***** DIURNAL RESPONSE RESULTS ***** UCTOLD *** DI Simulation terminated ***										
Reactor 3 Cycle number 2										
TIME	Zbh	Zba	Sads	Senm	VSS	Sbsc	Na	No3	TKN	Ot
0.0	2 570.1	84.4	60.6	3.3	4 128.3	0.0	0.3	12.2	3.4	51.6
2.0	2 496.2	82.7	48.2	3.4	4 026.2	0.0	0.3	11.7	3.0	46.1
4.0	2 446.0	82.1	44.3	3.3	3 976.0	0.0	0.4	11.6	3.7	45.5
6.0	2 525.4	85.9	67.2	3.5	4 150.5	0.0	0.8	12.3	5.1	65.0
8.0	2 596.4	88.8	97.0	3.5	4 289.8	0.0	1.4	14.3	6.0	80.8
10.0	2 624.7	89.5	112.6	3.6	4 329.6	0.0	1.3	16.1	6.2	83.3
12.0	2 630.8	89.2	112.6	3.5	4 317.5	0.0	1.2	17.6	6.4	81.6
14.0	2 630.7	88.7	108.3	3.5	4 295.3	0.0	0.9	18.6	5.6	77.0
16.0	2 654.3	88.9	116.1	3.4	4 321.1	0.0	0.8	18.1	5.1	76.5
18.0	2 670.7	88.7	113.3	3.5	4 327.2	0.0	0.6	16.6	4.7	72.5
20.0	2 674.9	88.0	103.4	3.5	4 313.0	0.0	0.5	14.6	3.9	66.8
22.0	2 643.3	86.4	81.7	3.4	4 242.5	0.0	0.4	12.5	3.8	59.1
24.0	2 579.0	84.4	60.7	3.3	4 135.5	0.0	0.3	11.4	3.4	51.7

Data set 2: UCTOLD Diurnal Simulation (TP code) with Accuracy% = 0.5 and Theta = 0.7



8.7. Discussion of comparative performance

The following table shows that the calculation time of UCTPHO is generally longer than for UCTOLD per the two UCT System test data sets, with integration parameters Accuracy%=1.0 and Theta=0.5:

SIMULATIONS	Time	SIMULATION DURATION		Time ratio
		UCTOLD	UCTPHO	UCTPHO/ UCTOLD
Data set 1				
Steady State Simulation	seconds	17	17	1
Diurnal Simulation	minutes	5.67	25.45	4.49
Data set 2				
Steady State Simulation	seconds	15	30	2
Diurnal Simulation	minutes	17.65	18.58	1.05

From this table it is seen that the calculation speed is specific to each data set. From 8.6 it is seen that the reduction in the Accuracy% value to 0.1 causes the duration of the calculation to increase drastically, from 5.67 min to 43 min in the case of UCTOLD for data set 1.

8.7.1. Data set 1

Both UCTPHO and UCTOLD in VBA correlated closely with the simulation results obtained from the TP software and the minor differences in the simulation results are ascribed to the accuracy parameters set prior to the calculations.

The concentration values of Zbh (heterotroph) and NO₃ (nitrates) are slightly higher in the VBA version than TP in the UCTOLD results. This seems to be linked to the Sads values (adsorbed COD), which is indicative that there may still be a minor error in the stoichiometry or process rate calculations. However, the discrepancy is minor and it is suggested that it would not make a significant difference in the simulation.

8.7.2. Data set 2

Although UCTPHO (VBA) results correlated closely with the TP results, there are still some minor discrepancies between the UCTOLD (VBA) diurnal results and the TP results as is seen with the comparison of the NO₃ concentrations in the results of the steady state simulations for data set 2. It is possible that these discrepancies are linked to the utilization of RBCOD, but Sub Stoichiometry as well as Sub ProcessRates were re-checked and no errors found.

For accuracy parameters set to the values of the TP code (Accuracy%=0.5, Theta=0.7, Data interval 15 min), the calculation time for UCTPHO increases from 18 min to 21 min after 2 integration cycles. There is also a minor improvement in the correlation with the results from the TP code.

9. CONCLUSION

The modelling with the Beta version is now complete and feedback by prospective users will provide useful information for the improvement of the software to make it more robust and user friendly.

The loss in computational speed as a result of using VBA instead of a more powerful programming language is believed to be at an acceptable level for this application since it provides free access to the software for consultants and operators that do not have resources or access to large budgets for the purchasing of costly modelling software for municipal wastewater treatment.

Testing to date indicates that a sufficient balance between accuracy and calculation speed is achieved by using the default parameters:

9.1. Steady state

Minimum output concentration = 0.01 g/m^3

9.2. Diurnal simulation

Integration parameters: Accuracy%=1.0 and Theta=0.5 for diurnal simulation with Data Interval = 15 minutes.

10. DISCLAIMER

The use of this software is permitted free of charge, but it is the responsibility of the user to use the software to supplement their thorough subject knowledge and not use the software as a substitute for subject knowledge. The normal rules for the responsible use of software must be applied and the relevant reliability checking performed when using software tools.

11. REFERENCES

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- Dold, PL, Wentzel, MC, Billing, AE, Ekama, GA, and Marais, GvR (1991). WRC Document TT 52/91: Nitrification and Nitrification/ Denitrification Systems Version 1.0
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ANNEXURE A: USER GUIDE

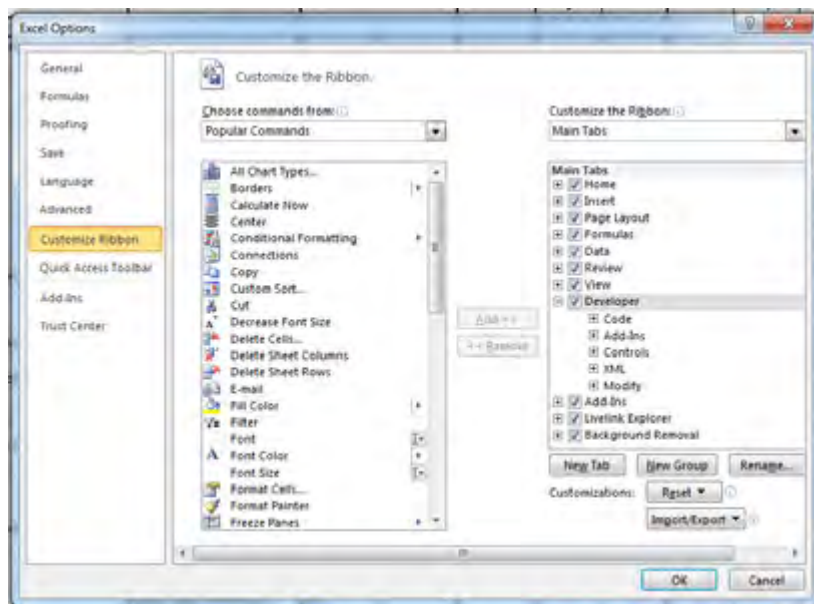
1. STARTING A PROJECT

The Excel file should be saved in its own folder. When the Excel file “UCTPHO UCTOLD 1 May 2016 Beta version Rev2” is uploaded, a sub folder (“OutputGIF”) is created where the simulation results per GIF image files are stored. At the start of the next project, these files are all deleted.

No adjustments are required to operate the program, but if some problems present themselves in this regard, the following should be confirmed:

1.1. Developer setting

In Excel Options/ Customize Ribbon, make sure “Developer” is ticked.



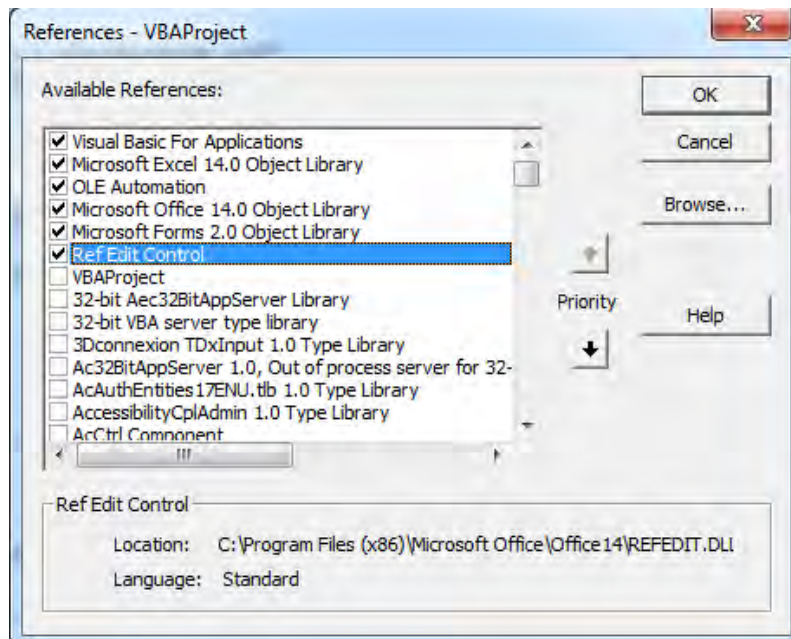
If this is ticked, “Developer” will be visible in the top ribbon in Excel.

1.2. References

The relevant references have to be selected. However, it should not be necessary to make any changes since these references were selected in the development of the program.

In Excel press Alt-F11 to get to VBA. Alternatively Click on Developer in the top ribbon in Excel, then Visual Basic. This opens the Visual Basic for Applications (Excel) Main Menu or the VBE Main Menu.

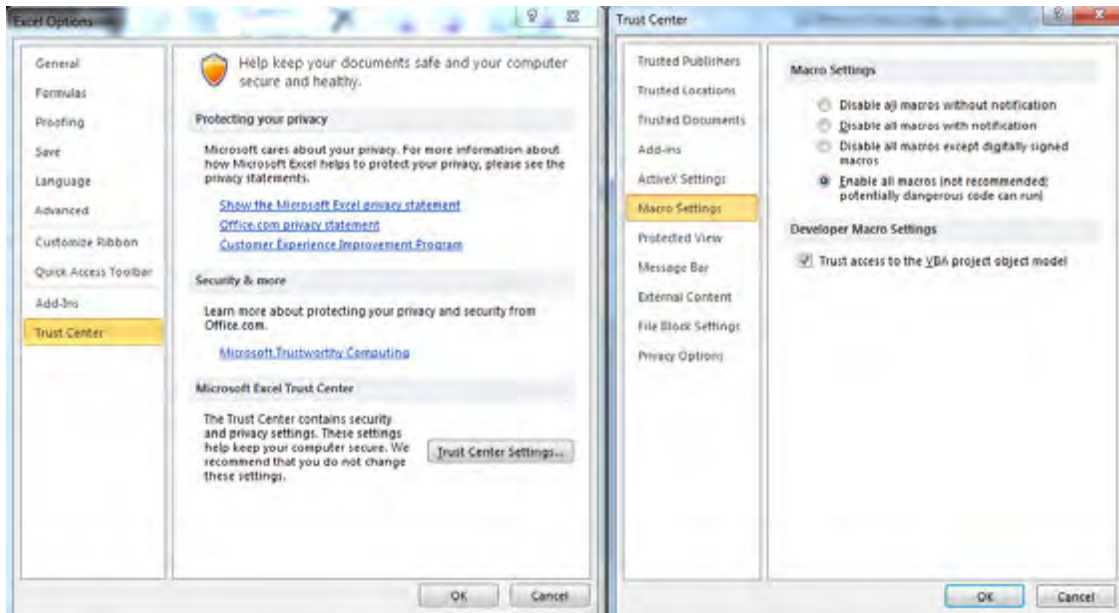
In the main VBE window, select Tools/ References and make sure the following are ticked:



- Visual Basic For Applications
- Microsoft Excel 14.0 Object Library
- OLE Automation
- Microsoft Office 14.0 Object Library
- Microsoft Forms 2.0 Object Library
- Ref Edit Control
- Microsoft Visual Basic for Applications Extensibility 5.3

1.3. Macro setting

Also ensure that Macros are enabled:

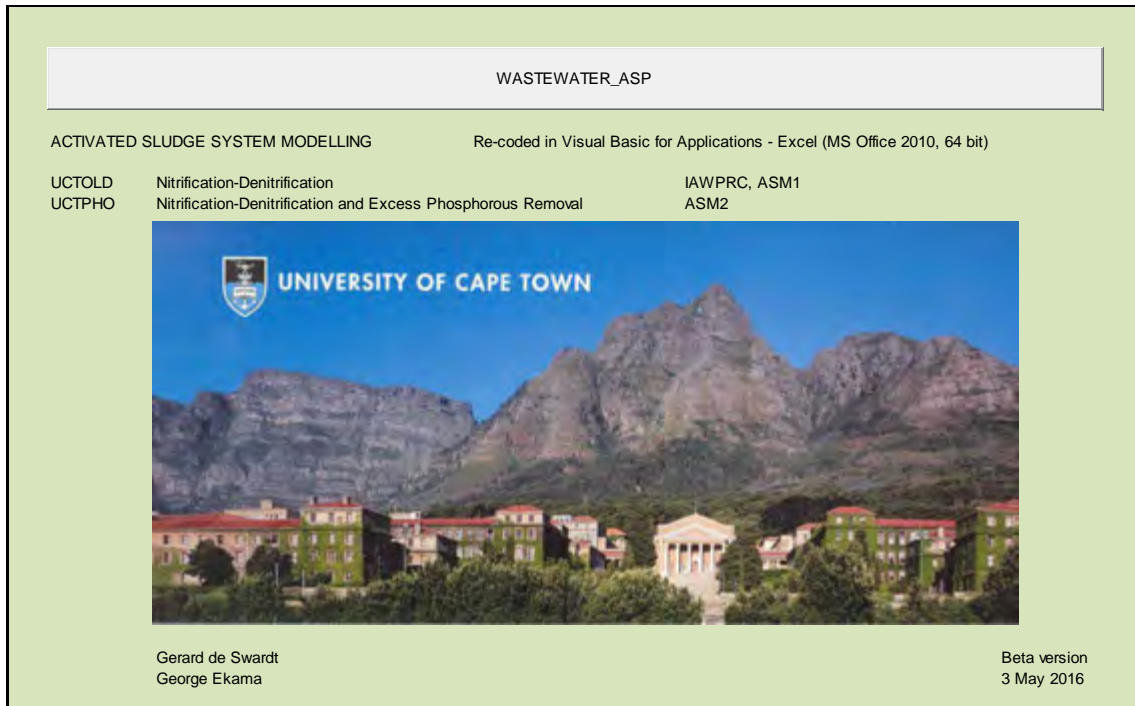


Once this is done, proceed with the data input in the user interface.

2. USER INTERFACE

The user interface of the original Turbo Pascal version was outdated and warranted certain improvements for data entry and project setup.

The start-up screen is found on the tab “StartPage”. The program runs when the button “WASTEWATER_ASP” is clicked:



The Excel sheet tabs are colour coded as follows:

TAB KEY

INPUT
OUTPUT
CALCULATIONS
PASCAL CODE
FLOWCHART

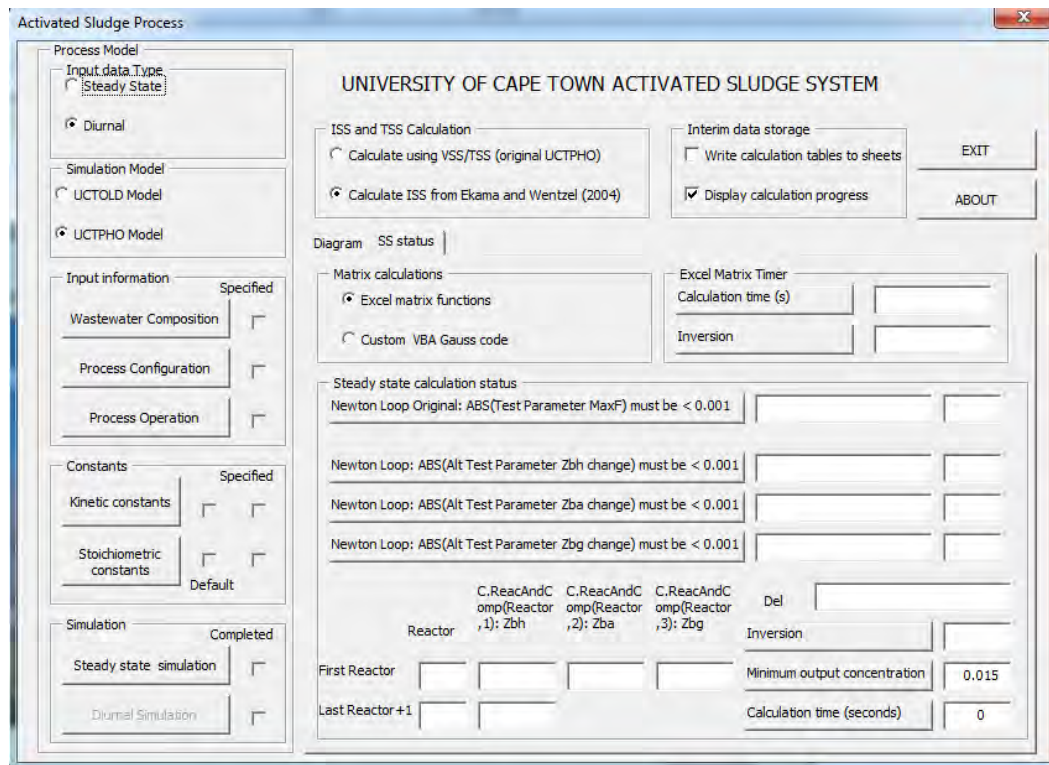
Annexure C shows a flow diagram of the program operation. All actions are accessed from the main menu and the simulation steps have to be followed in sequence.

2.1. Input

Input tables provide an overview of each parameter set and an easy way to edit default values for a specific project.

The main menu is displayed and the input parameters can now be entered before simulation of the system.

The user only needs to deal with the frame “Process Model” and follow the buttons in sequence to complete a process simulation:



The input data type needs to be selected by checking the relevant Option button in the “Input data type” frame. The options are Steady State and Diurnal.

In the Simulation Model frame, option buttons are displayed for UCTOLD model and UCTPHO model to be selected.

The ISS calculation method could also be specified in the frame “ISS and TSS Calculation”, but the default is the newly incorporated method per Ekama and Wentzel (2004).

2.2. Water quality & characterization

Select the button “Wastewater Composition”. The input table requires water quality and flow information to be entered. For Steady State, only one value is required for

each parameter. When Diurnal is selected on the Main menu, flow and quality data is required at 2 hour intervals over a 24 hour period.

Input water quality parameters are COD, TKN and P in g/m³ or mg/l. Flow is entered in m³/d or in m³/h. An option was added to input data for VSS and TSS or a ratio for input VSS/TSSi ratio for the purpose of modelling the influent ISS through the system.

It is good practice to overwrite values rather than deleting first and typing new values in. Although an effort has been made to reduce errors by data validation, some errors may still occur when data entry text boxes are emptied before data is entered, and this will have to be addressed as errors are encountered.

INFLUENT WASTEWATER DATA INPUT

Flow rate (m³/day) COD (g/m³) TKN (g/m³) P (g/m³) VSS (g/m³) TSS (g/m³)

Average flows and concentrations
 FLOW WEIGHTED AVERAGE (g/m³)

Flow rate (m ³ /day)	COD (g/m ³)	TKN (g/m ³)	P (g/m ³)	VSS (g/m ³)	TSS (g/m ³)
24080	1058.083	81.1	18.367	451.483	610.333

Wastewater
 Raw
 Settled
 Fractions

Diurnal intervals

Record number	Time (h)
1	0
2	2
3	4
4	6
5	8
6	10
7	12
8	14
9	16
10	18
11	20
12	22

Diurnal flows and concentrations

Rate	COD (g/m ³)	TKN (g/m ³)	P (g/m ³)
<input type="checkbox"/> m ³ /hour			
<input checked="" type="checkbox"/> m ³ /day			
8640	445	37.5	8
11904	353	60	6
36288	843	87.1	14.5
41472	1955	102.1	20.9
34960	1304	112.6	23.1
28032	1334	121.6	24.1
24576	1472	102.6	26.7
27840	1380	93.1	23.7
25526	1303	84.1	21.6
23232	1227	83	19.9
16320	1120	60	19.1
10560	751	49.5	12.8

Influent VSS and TSS data
 Data input VSS/TSS ratio input

VSS and TSS	VSS (g/m ³)	TSS (g/m ³)
154.7	221	
182.25	243	
496	620	
531.2	664	
566.4	708	
584	752	
630.75	841	
557.9	797	
511	730	
495.6	708	
449.4	642	
278.6	398	

AS TSS Calc.
 VSS/TSS input for AS
 Calculate TSS per Ekama/Wentzel 2004

Alkalinity
 Influent Alkalinity (mol/m³)
 10 (g/m³)
 500

OK REFRESH CANCEL Help

In the Wastewater frame, Raw or Settled wastewater is selected. From here, the characterisation parameters can be adjusted by clicking on the “Fractions” button. This data is stored on sheet “InputData”.

2.3. Raw

From this screen, the default values could be accepted or changed:

EDIT WASTEWATER FRACTIONS

Raw

Raw wastewater fractions

1	Fbs	Biodegradable soluble (readily biodegradable)	0.2
2	Fac	Short chain fatty acid (readily biodegradable COD)	0.1
3	Fus	Unbiodegradable soluble fraction of COD	0.05
4	Fup	Unbiodegradable particulate fraction of COD	0.13
5	FupP	Unbiodegradable particulate P fraction of COD	0.014
6	Fna	Ammonia fraction of TKN	0.75
7	Fnobp	Biodegradable particulate organic N	0.5
8	Fnous	Unbiodegradable soluble organic N	0.03
9	Fzbh	Fraction of influent COD that is heterotrophs	0
10	VSS/ TSS ratio (activated sludge)		0.75
11	VSS/ TSS ratio (influent wastewater)		0.75

ISS P parameters

12	FusP	Unbiodegradable soluble P fraction of COD	0
13	UPO fp	Fraction P of VSS	0.025

Input fraction:

Default values
 Changed values

OK
 Cancel
 Help

ISS in biomass

f_{iOHO} (g ISS/g OHO COD)
 0.1

f_{iOHO} (g ISS/g OHO VSS)
 0.15

The option button “Changed values” has to be selected before changes to parameter values will be allowed.

The ISS ratio of the biomass (f_{iOHO}) is entered either here or on the Stoichiometric menu.

2.4. Settled

From this screen, the default values could be accepted or changed.

Settled wastewater fractions			
1	Fbs	Biodegradable soluble (readily biodegradable)	0.3
2	Fac	short chain fatty acids (readily biodegradable COD)	0.1
3	Fus	Unbiodegradable soluble fraction of COD	0.08
4	Fup	Unbiodegradable particulate fraction of COD	0.04
5	FupP	Unbiodegradable particulate P fraction of COD	0.014
6	Fna	Ammonia fraction of TKN	0.83
7	Fnobp	Biodegradable particulate organic N	0.5
8	Fnous	Unbiodegradable soluble organic N	0.04
9	Fzbh	Fraction of influent COD that is heterotrophs	0
10	VSS/ TSS ratio (activated sludge)		0.83
11	VSS/ TSS ratio (influent wastewater)		0.83

ISS P parameters			
12	FusP	Unbiodegradable soluble P fraction of COD	0
13	UPO fp	Fraction P of VSS	0.025

Input fraction:
 Default values
 Changed values

OK
 Cancel
 Help

ISS in biomass

f_{iOHO} (g ISS/ g OHO COD)
 0.1

f_{iOHO} (g ISS/ g OHO VSS)
 0.15

The option button “Changed values” has to be selected before changes to parameter values will be allowed.

The ISS ratio of the biomass (f_{iOHO}) is entered either here or on the Stoichiometric menu.

2.5. Process selection/ Configuration

Select button “Process Configuration”. The input in the user interface is done as follows:

2.5.1. User Input

By clicking on the Process Configuration button on the Main Menu invokes the following screen:

One of the process configurations can be selected in the Process option frame. There is an option for Custom process if the included options are inadequate.

In the Recycle selection frame it is required that either the ratio or the flow rate of each recycle be specified. A, B and RAS (a, r and s) recycle options are provided.

The reactor sizes must be entered in the Reactors frame. The aeration state, dissolved oxygen concentration (mg/l) and influent flow fraction must also be specified for each reactor.

The process schematic is displayed at the bottom for any of the library process types. No diagram is displayed for a custom process type.

This input data is stored on sheet "InputData".

2.5.2. Reactor Numbering Convention (Appendix C of Dold et al. (1991))

The structure of the program requires that the reactors in the system configuration are numbered using a defined procedure. This procedure should be followed when entering the Plant Configuration data:

- Draw the number of reactors in the system in a linear sequence following the stream of flow from reactor to reactor.
- The secondary clarifier is positioned at the downstream end of the reactor sequence.
- Number the reactors in descending order backwards, assigning the reactor immediately upstream of the clarifier with the highest number. The reactor furthest upstream of the clarifier will then be assigned number 1. The program assumes that inter-reactor flow passes sequentially from reactor to reactor (starting at No.1) towards the clarifier without bypassing any reactor in the sequence.
- Not more than one clarifier underflow recycle and two mixed liquor recycles can be modelled, and each can only enter one reactor. Membrane systems can be modelled by returning the clarifier underflow to the reactor immediately before it.
- The mixed liquor recycles can have any reactor as point of origin but must discharge into a reactor upstream of the point of origin; that is, the reactor number of the point of origin must be greater than the reactor number of the point of discharge.
- The influent flow can discharge into any reactor in the series, or be split between a number of reactors.
- The program allows simulation of systems with reactors in the underflow (RAS) recycle (e.g. the JHB system) provided these reactors are at the start of the reactor sequence and the influent enters the system downstream of the underflow reactor(s). The program cannot simulate systems with reactors between the point of origin and discharge of the mixed liquor recycles, i.e. no reactors are allowed in the mixed liquor recycles.

Examples illustrating the reactor numbering convention are set out in Appendix C of Dold et al. (1991).

2.6. Process Operation

The operating parameters have to be specified here. Sludge age in days and temperature in degrees Celsius are required. The recycle flows are displayed again and could also be edited here.

Operating parameters	
Sludge age/ SRT: Rs (days)	10
Process temperature: T (deg C)	22
Average influent flow (m3/d)	24080
A-recycle flow (m3/d)	72240
B-recycle flow (m3/d)	24080
RAS-recycle flow (m3/d)	24080

Buttons: OK, Cancel, Help

This data is stored on sheet “InputData”.

2.7. Kinetic Constants

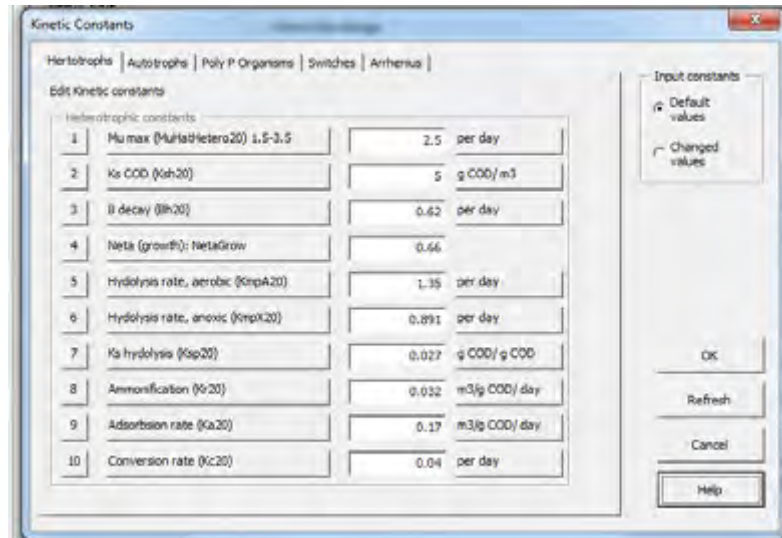
Kinetic constants can be entered here. Default values are displayed and could be accepted or changed. This data is stored on sheet “Parameters”.

All the kinetic constants are grouped together on a single screen with a multi page selector for the respective constant collection.

This data is stored on sheet “Parameters”.

2.7.1. Heterotrophs

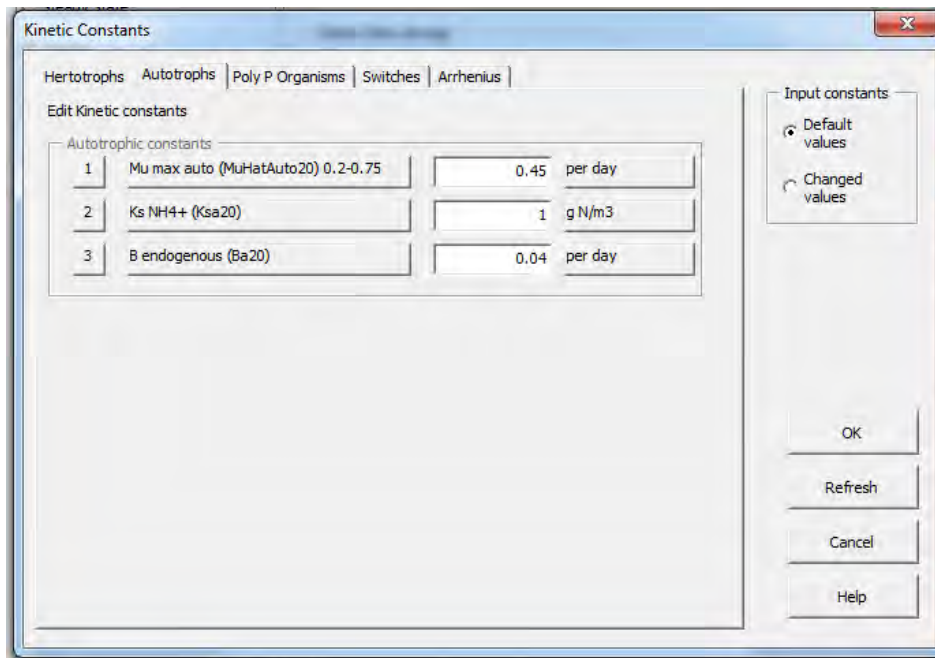
The heterotrophic constants frame displays the default values that can be accepted on clicking OK, or values can be changed and will be saved when clicking the OK button.



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.7.2. Autotrophs

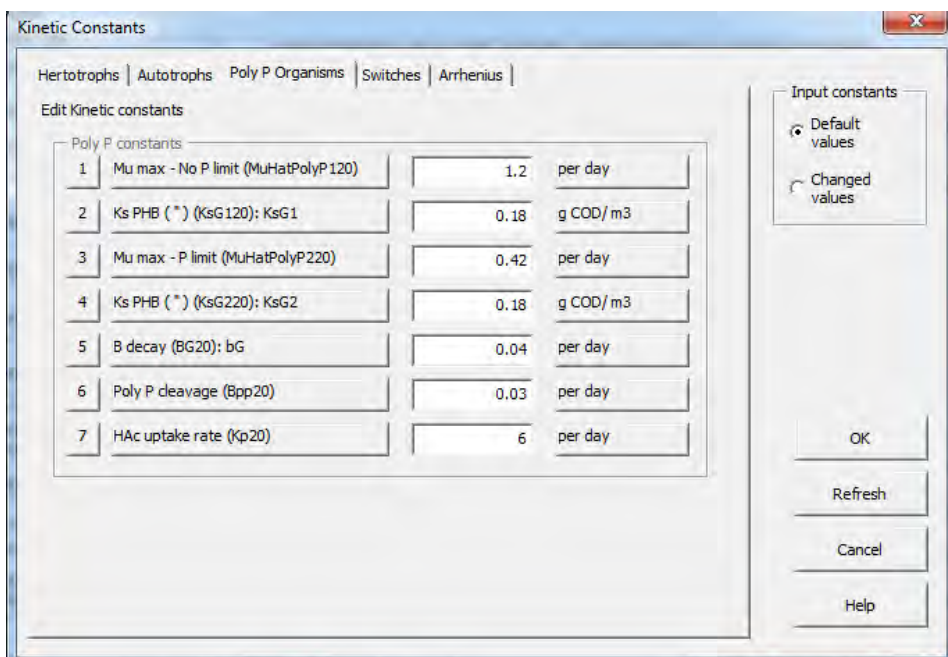
The autotrophic constants frame displays the default values that can be accepted on clicking OK, or values can be changed and will be saved when clicking the OK button.



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.7.3. P Organisms

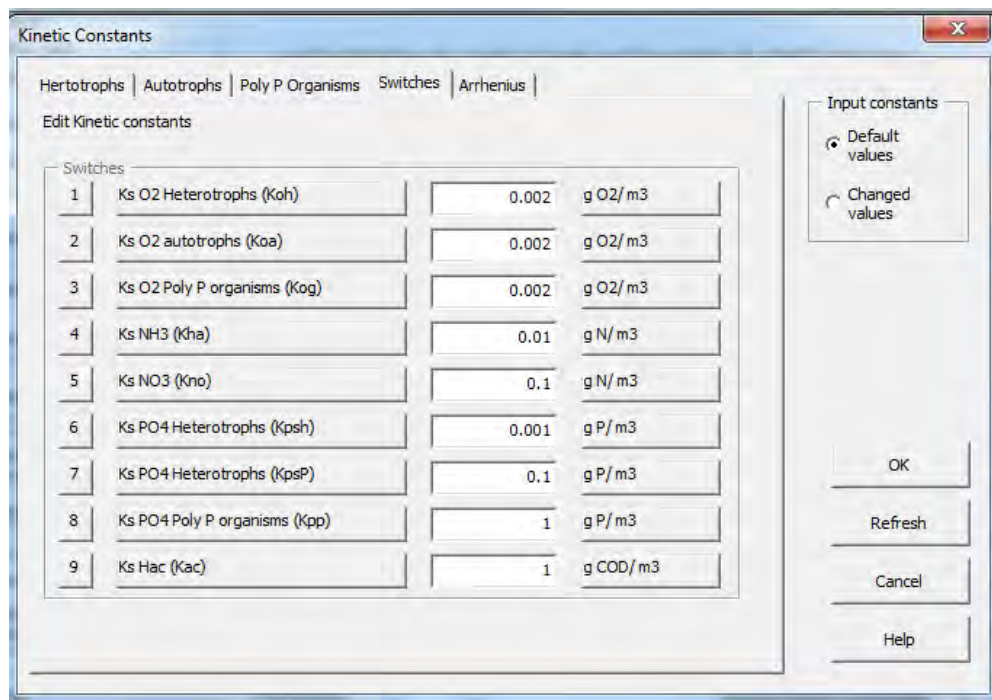
The Poly P constants frame displays the default values that can be accepted on clicking OK, or values can be changed and will be saved when clicking the OK button.



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.7.4. Switches

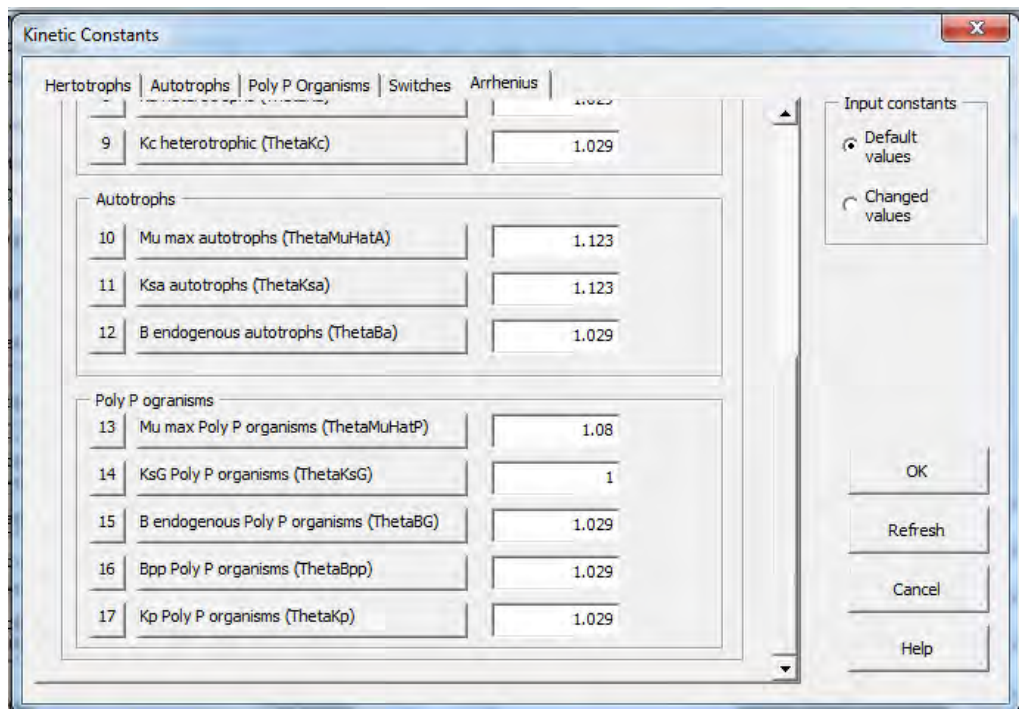
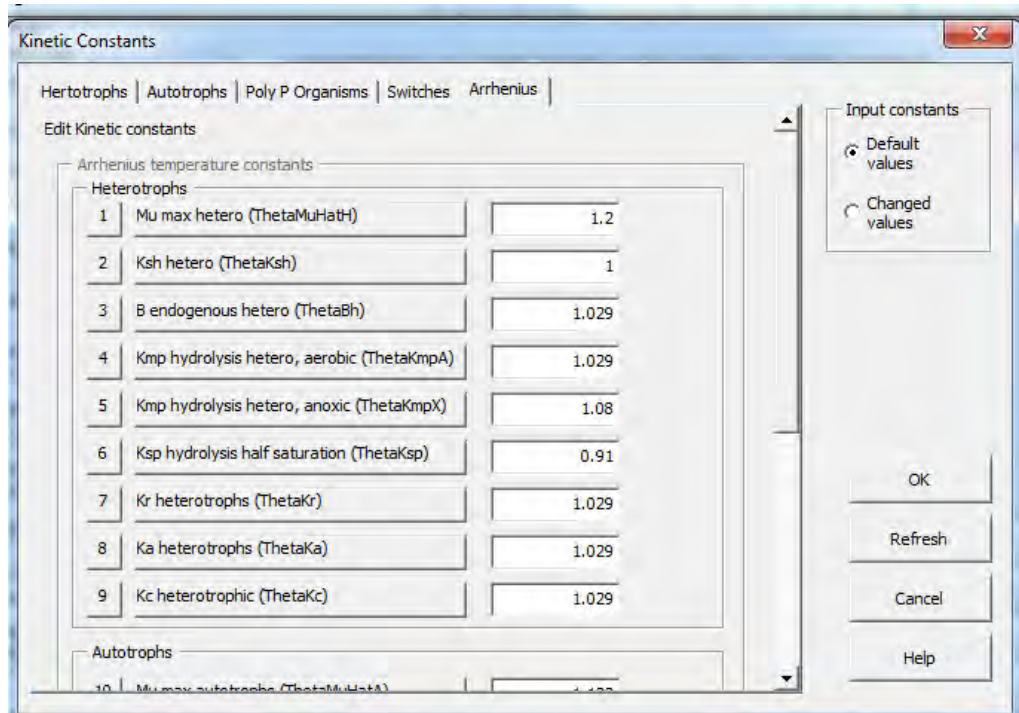
The Switches frame displays the default values that can be accepted on clicking OK, or values can be changed and will be saved when clicking the OK button.



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.7.5. Arrhenius

The Arrhenius temperature constants frame displays the default values that can be accepted on clicking OK, or values can be changed and will be saved when clicking the OK button.



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.8. Stoichiometric Constants

Stoichiometric constants can be entered here. Default values could be accepted or changed. This data is stored on sheet “Parameters”.

This data is stored on sheet “Parameters”.

2.8.1. Heterotrophs

Heterotrophic constants			
1	Yield (Yzh)	0.666	g COD/g COD
2	Frac inert particulate (Feph)	0.08	g COD/g COD
3	Max ads/ hetero (fma)	1	g COD/g COD
4	N in biomass (Fzbhn)	0.068	g N/g COD
5	N in enogenous (Fzehn)	0.068	g N/g COD
6	P in biomass (Fzbhp)	0.02	g P/g COD
7	P in endogenous (Fzelp)	0.02	g P/g COD
8	COD: VSS ratio	1.48	g COD/g VSS

ISS content of Heterotrophs, Autotrophs and Poly P Organisms

9	Biomass ISS content (fioHO)	0.1	g ISS/g COD
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The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.8.2. Autotrophs

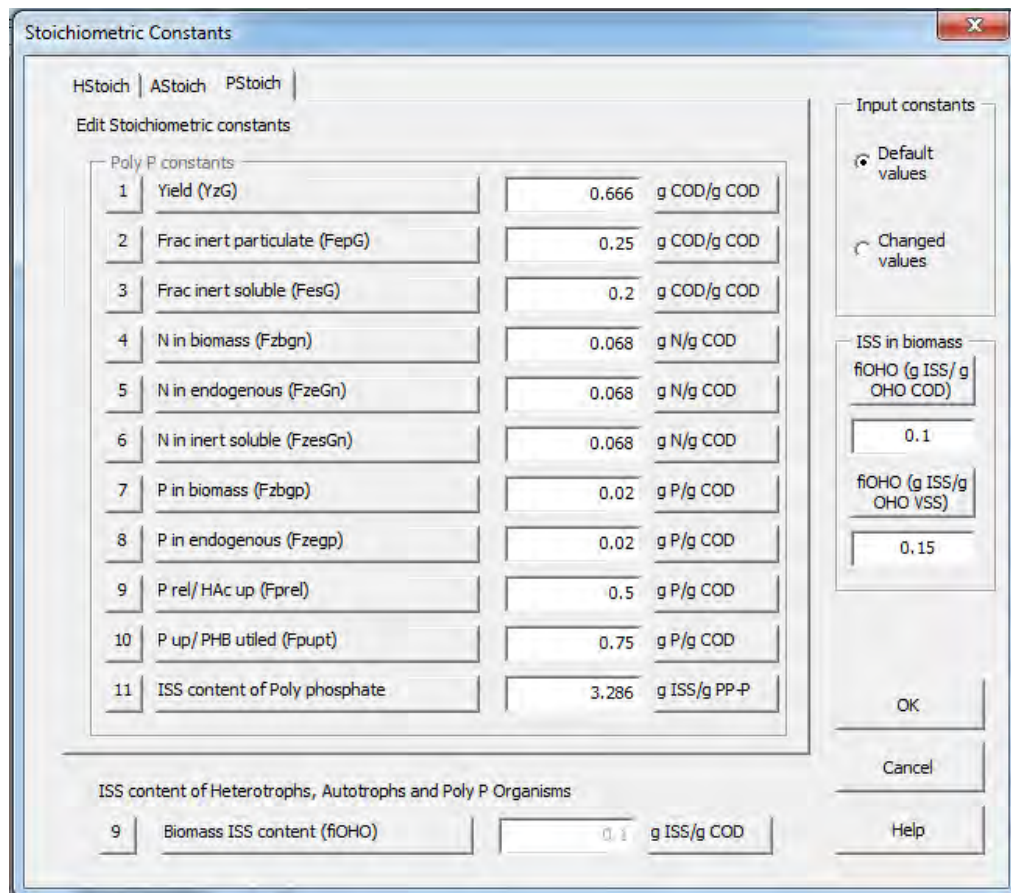
Parameter	Value	Unit
1 Yield (Yza)	0.15	g COD/g COD
2 Frac inert particulate (FepA)	0.08	g COD/g COD
3 N in biomass (Fzban)	0.068	g N/g COD
4 N in endogenous (Fzean)	0.068	g N/g COD
5 P in biomass (Fzbap)	0.02	g P/g COD
6 P in endogenous (Fzeap)	0.02	g P/g COD

ISS content of Heterotrophs, Autotrophs and Poly P Organisms

Parameter	Value	Unit
9 Biomass ISS content (fIOHO)	0.1	g ISS/g COD

The option button “Changed values” has to be selected before changes to parameter values will be allowed.

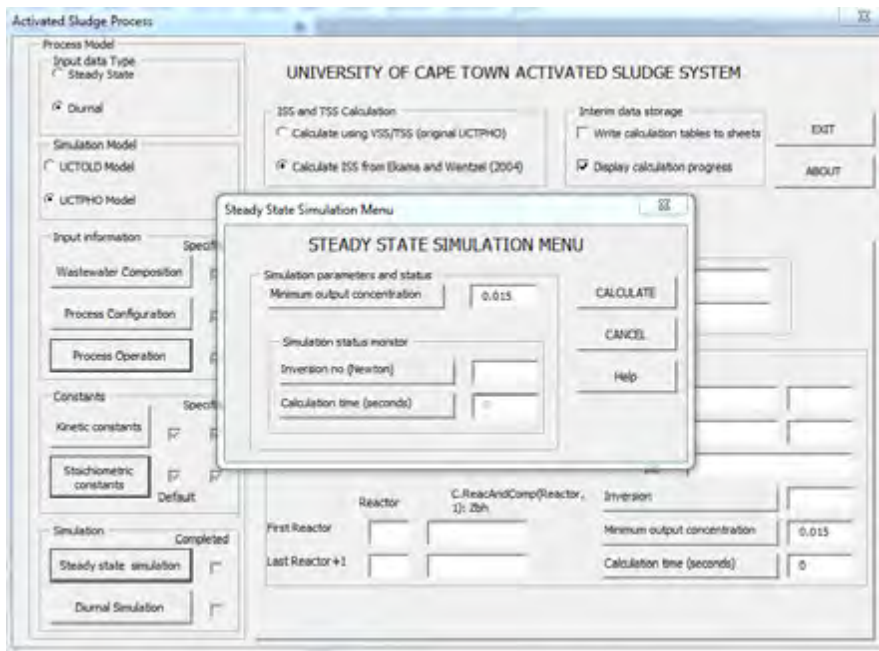
2.8.3. Poly P Organisms



The option button “Changed values” has to be selected before changes to parameter values will be allowed.

2.9. Steady State Simulation

The steady state simulation is invoked from the main menu, only after the first five steps (Wastewater composition, Process Configuration, Process Operation, Kinetic Constants) have been completed.

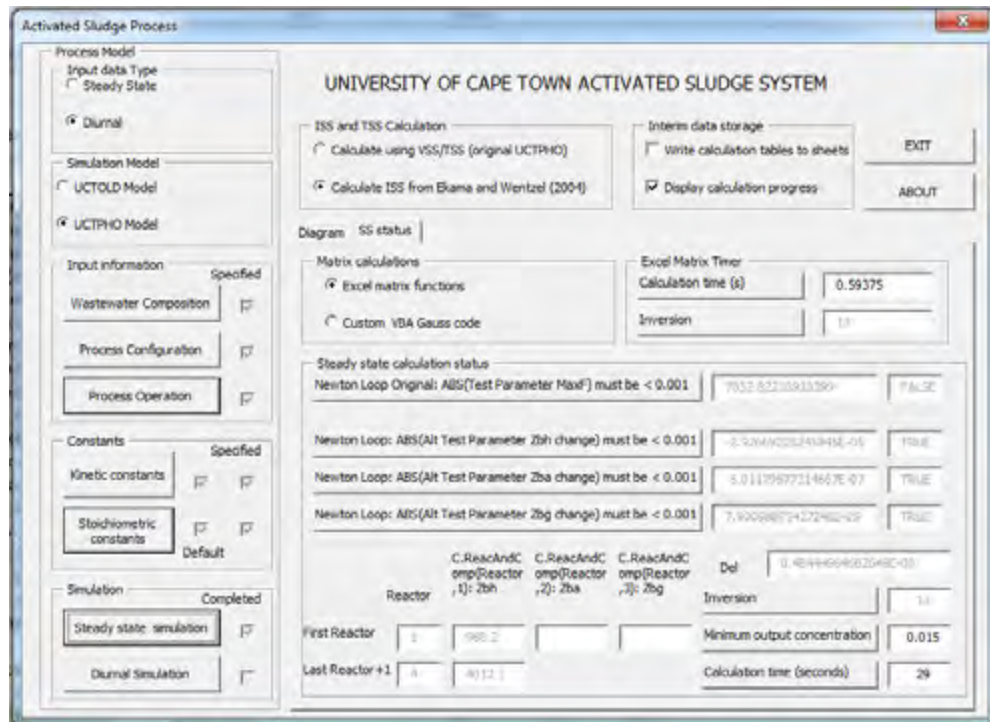


The frame “Simulation parameters and status” displays the status of the steady state simulation. This was included due to the longer calculation time compared to Turbo Pascal to indicate when the iteration parameters are satisfied and what the calculation duration was. The only variable that can be changed here is the minimum output concentration with a default value of 0.010.

STEADY STATE RESULTS: UCTPHO, ISS calc: Ekama & Wentzel (2004), Inversions = 13, Calculation time = 28 seconds						
COMPOUND	UNIT	INPUT	REACTOR	1	2	3
1	Zbh (betens.)	g COD m-3	0.0	968.2	2 038.1	2 078.1
2	Zba (auto.)	g COD m-3	0.0	36.2	72.8	73.9
3	Zbg (polyP org.)	g COD m-3	0.0	376.9	757.1	769.0
4	Zb (endog. COD)	g COD m-3	0.0	574.4	1 137.3	1 149.0
5	Zi (inert. COD)	g COD m-3	137.6	1 062.1	1 986.6	1 986.6
6	Sads (adsorbed COD)	g COD m-3	0.0	468.3	204.6	68.5
7	Senm (enmeshed COD)	g COD m-3	594.1	39.9	6.0	3.5
8	Sphb (PHB COD)	g COD m-3	0.0	82.6	60.0	27.2
9	Nobp (prt bio N)	g N m-3	4.2	9.0	5.6	2.9
10	Ppp (stored polyP)	g P m-3	0.0	37.7	136.1	150.9
11	ISSi (influent ISS)	g ISS m-3	158.9	1 226.5	2 294.2	2 294.2
12	Sbs.c (compt RBCOD)	g COD m-3	156.2	12.2	0.1	0.1
13	Sbs.a (SCFA RBCOD)	g COD m-3	17.4	0.3	0.1	0.1
14	Na (ammonia N)	g N m-3	60.8	37.7	12.3	0.7
15	Nobs (sol org N)	g N m-3	4.24	0.64	1.14	1.56
16	No3 (nitrate N)	g N m-3	0.0	0.1	5.1	14.6
17	Pa (soluble P)	g P m-3	16.4	47.8	16.4	0.4
18	Sus. (sol unbr COD)	g COD m-3	52.9	55.1	56.7	57.3
19	Alkalinity	mole m-3	10.0	8.5	6.5	5.0
Volatile SS			g VSS m-3	2 438.2	4 224.7	4 159.4
Total SS			g TSS m-3	3 926.7	7 253.0	7 241.6
OUR carbonaceous			g O2 m-3 h-1	0.0	0.0	43.6
OUR autotrophs			g O2 m-3 h-1	0.0	0.0	17.9
OUR total			g O2 m-3 h-1	0.0	0.0	61.7
Denitr. rate			g NO3-N m-3 h-1	12.5	13.8	0.1
TKN			g TKN m-3 h-1	40.5	14.9	3.2

This example shows that the calculation time for the steady state simulation was 28 seconds.

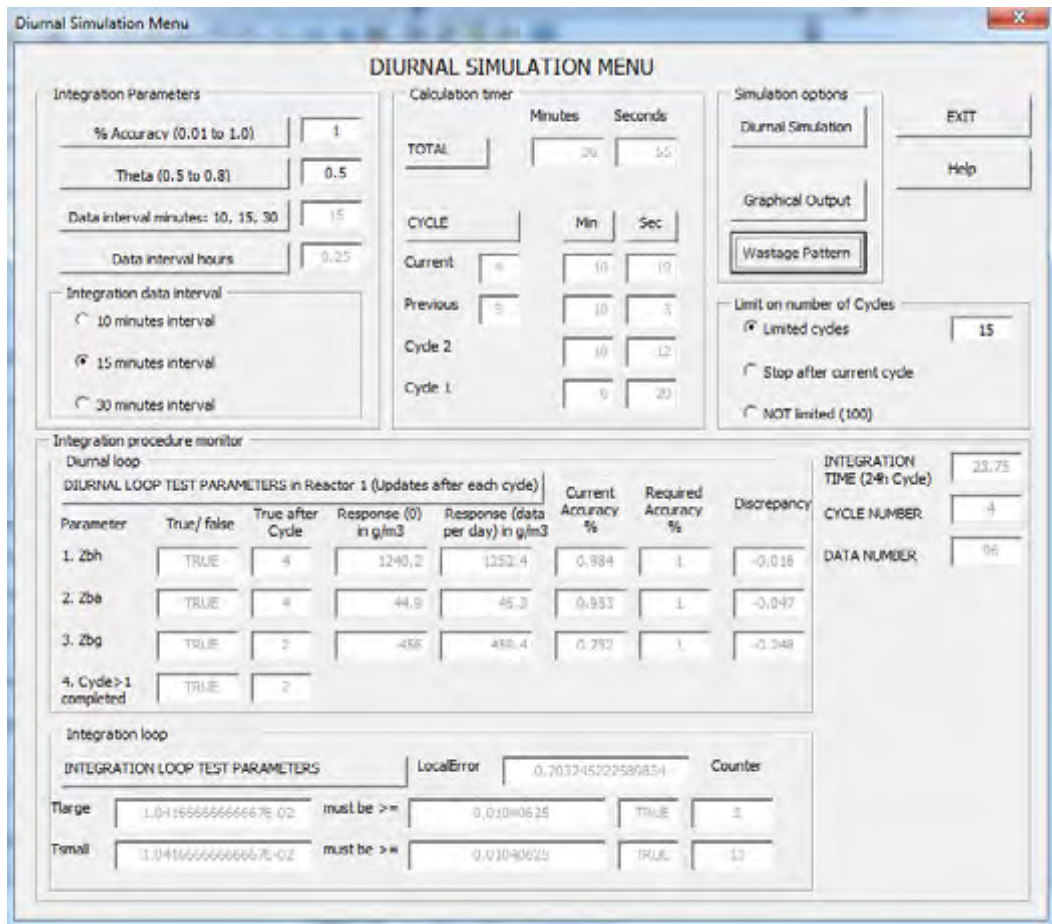
This screen displays the accuracy of the three test parameters as well as the calculation time.



2.10. Diurnal Simulation

The frame “Integration parameters” does not require adjustment of the parameters, but adjustment can be made to the two parameters if required.

The diurnal simulation is started by clicking on the button “Diurnal Simulation” in the frame “Simulation Options”.



The frame “Integration procedure monitor” displays the progress in the calculation loops in the software. The Integration loop parameters are constantly updated and the Diurnal loop parameters are updated after the integration has been completed for each calculation cycle of 24 hours.

The section “Diurnal loop parameters” provides valuable information so that the user can assess calculation progress and the current accuracy achieved while following the Integration time (24h Cycle).

The frame “Calculation timer” displays the Total calculation time as well as the time taken per cycle. It is noted that each cycle does not take the same time to calculate.

In the “Diurnal loop” frame, the information on the current accuracy of three test parameters is displayed and also the cycle number when that parameter test value became true. If the user feels that the calculation time is becoming too long, a decision could be made to terminate the simulation if it is felt that the accuracy is approaching an acceptable level. There are three options to choose from in the frame “Limit on number of Cycles”.

The diurnal response for each calculation cycle is written to sheet “Dresponse” and that of the last reactor is displayed on completion of the diurnal simulation:

***** DIURNAL RESPONSE RESULTS *****UCTPHO
 Reactor 3 Cycle number 4

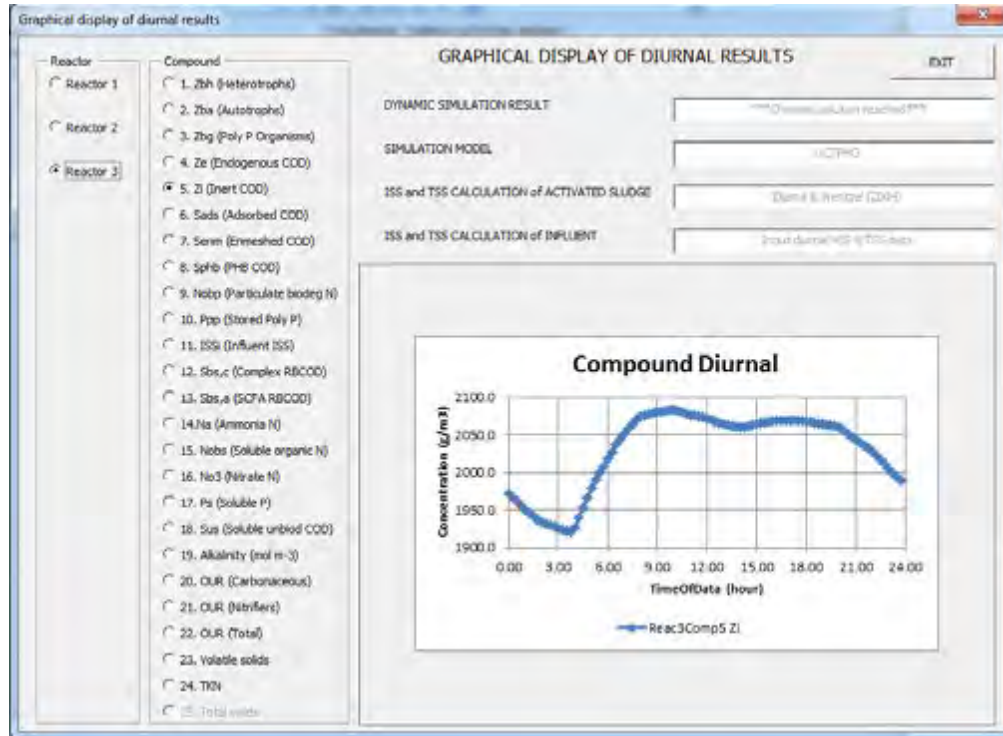
TIME	Zbh	Zba	Zbg	Sads	Sphb	Ppp	Sbcb	No3	Ps	Or
0.0	2 183.5	74.5	753.1	52.6	30.4	143.8	0.0	13.7	0.1	46.6
2.0	2 122.1	72.9	748.6	40.6	26.5	140.6	0.0	12.3	0.1	41.0
4.0	2 080.1	72.3	743.4	36.8	22.8	139.5	0.0	11.3	0.1	40.6
6.0	2 148.5	75.8	775.9	56.7	22.1	146.1	0.0	11.7	0.4	51.0
8.0	2 208.3	78.5	797.5	85.6	25.4	149.1	0.0	14.5	2.0	77.7
10.0	2 231.5	79.3	801.0	102.4	31.2	148.8	0.0	17.7	2.9	81.1
12.0	2 235.8	79.2	797.7	103.6	33.6	148.5	0.0	20.3	2.1	79.4
14.0	2 237.9	78.9	793.6	99.6	34.2	148.5	0.0	21.8	0.8	74.7
16.0	2 259.4	79.2	795.5	105.9	35.0	149.2	0.0	21.8	0.7	74.2
18.0	2 275.4	79.0	797.0	104.1	35.7	149.4	0.0	20.6	0.4	69.7
20.0	2 281.4	78.5	794.9	94.2	35.4	148.6	0.0	18.4	0.2	63.4
22.0	2 257.1	77.1	784.5	73.0	34.0	146.6	0.0	15.9	0.1	54.9
24.0	2 204.2	75.2	768.8	52.6	30.7	143.2	0.0	13.8	0.1	47.0

Finally, the reactor concentrations are displayed at the end of the simulation:

DIURNAL RESULTS: UCTPHO, ISS calc: Ekama & Wentzel (2004); Cycles = 4. Runtime = 37.15 minutes and *** Dynamic solution reached***

No	COMPOUND	UNIT	REACTOR		
			1	2	3
1	Zbh (hetero.)	g COD m-3	1252.3	2111.4	2204.3
2	Zba (auto.)	g COD m-3	45.3	72.5	75.2
3	Zbg (polyP org.)	g COD m-3	459.7	739.5	768.8
4	Ze (endog COD)	g COD m-3	690.9	1 093.6	1 130.9
5	Zi (inert COD)	g COD m-3	1 269.2	1 937.0	1 989.4
6	Sads (adsorbed COD)	g COD m-3	462.6	154.0	52.6
7	Senm (enmeshed COD)	g COD m-3	12.4	4.4	3.4
8	Sphb (PHB COD)	g COD m-3	75.5	45.8	30.6
9	Nobp (prt bio N)	g N m-3	10.1	4.9	2.6
10	Ppp (stored polyP)	g P m-3	56.1	129.3	143.2
11	ISSi (influent ISS)	g ISS m-3	1 425.5	2 172.3	2 230.9
12	Sbs,c (compl RBCOD)	g COD m-3	1.9	0.0	0.0
13	Sbs,a (SCFA RBCOD)	g COD m-3	0.0	0.0	0.0
14	Na (ammonia N)	g N m-3	23.9	6.3	0.3
15	Nobs (sol org N)	g N m-3	0.3	1.2	1.5
16	No3 (nitrate N)	g N m-3	0.0	5.9	13.8
17	Ps (soluble P)	g P m-3	39.99	11.45	0.08
18	Sus (sol amb COD)	g COD m-3	60.3	64.1	65.2
19	Alkalinity	mole m-3	7.7	5.7	4.6
23	Volatle solids	g VSS m-3	2 883.8	4 160.9	4 226.5
25	Total solids	g TSS m-3	4 669.3	7 050.4	7 232.9
20	OUR carb	g O2 m-3 h-1	0.0	0.0	37.0
21	OUR nitr	g O2 m-3 h-1	0.0	0.0	37.0
22	OUR tot	g O2 m-3 h-1	0.0	0.0	47.0
26	Denitrification rate	g NO3-N m-3 h-1			
24	TKN	g N m-3	25.6	8.9	3.3

On completion of the diurnal simulation, the “Graphic Display” button is enabled and if clicked, it opens the following screen:



The reactor could be selected here as well as the compound for which a graph of the diurnal concentration pattern is required. This will display the graph on the screen as shown in this example.

Each graph that is viewed is saved as a .GIF file in the sub folder “OutputGIF” and will be accessible until a next simulation is started, when the .GIF files are all deleted.

Selection of the button “Wastage Pattern” opens this screen:

The dialog box 'Check or change wastage pattern' is titled 'WASTAGE PATTERN'. It contains the following sections:

- Mean flow:** Mean flow (m³/day) with input fields for 24080 and 1667.31.
- Resulting sludge age:** Actual (days) set to 11.4 and Required (days) set to 10.
- Diurnal intervals:** A table with columns 'Record number' and 'Time (h)'.

Record number	Time (h)
1	0
2	2
3	4
4	6
5	8
6	10
7	12
8	14
9	16
10	18
11	20
12	22
- Influent flow Rate:** Radio buttons for m³/hour and m³/day.
- Wastage flow Rate:** Radio buttons for m³/hour and m³/day.
- Input flow rates:** Radio buttons for Default values and Changed values.
- Wastage Switches:** Number of Waste intervals set to 12. A list of 12 intervals, each with 'On' and 'Off' radio buttons.
- Buttons:** OK, CANCEL, and Help.

Wastage could be switched on or off as required and then the flow rates will be adjusted to still apply the same sludge age as before.

The results are displayed on the Excel sheets where the tab colour is green. From these sheets the results can be copied and manipulated as required for presenting in reports.

ANNEXURE B: DEFAULT CONSTANTS (from TP code)

UCTPHO	UCTOLD
FRACTIONATION CONSTANTS	
Procedure Settled;	Procedure Settled;
Fbs := 0.30;	Fbs := 0.25;
Fac := 0.10;	
Fus := 0.08;	Fus := 0.08;
Fup := 0.04;	Fup := 0.04;
FupP := 0.014;	
Fna := 0.83;	Fnaa := 0.83;
Fnobp := 0.50;	Fnox := 0.50;
Fnous := 0.04;	Fnu := 0.04;
Fzbh := 0.0;	Fxbh := 0.0;
VSSTSS := 0.83;	VSSTSS := 0.83;
Procedure Raw;	Procedure Raw;
Fbs := 0.20;	Fbs := 0.20;
Fac := 0.10;	
Fus := 0.05;	Fus := 0.05;
Fup := 0.13;	Fup := 0.13;
FupP := 0.014;	
Fna := 0.75;	Fnaa := 0.75;
Fnobp := 0.50;	Fnox := 0.50;
Fnous := 0.03;	Fnu := 0.03;
Fzbh := 0.0;	Fxbh := 0.0;
VSSTSS := 0.75;	VSSTSS := 0.75;
KINETIC CONSTANTS	
{Heterotrophs}	
MuHatHetero20 := 2.5; {Mu max}	MuHatHetero20 := 3.2;

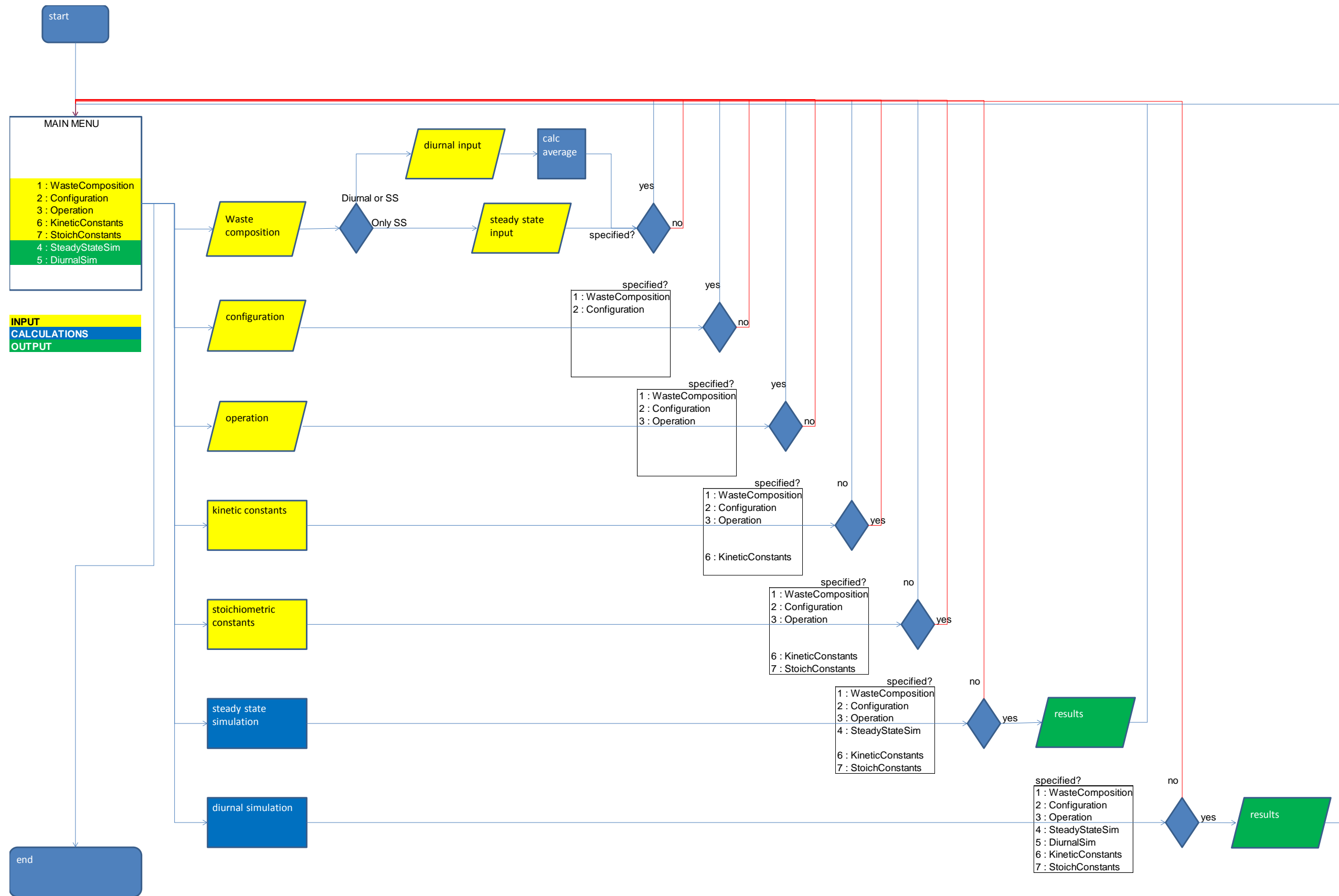
UCTPHO	UCTOLD
Ksh20 := 5.0; {Ks COD}	Ks20 := 5.0;
Bh20 := 0.62; {B decay}	Bh20 := 0.62;
NetaGrow := 0.66; {Neta (growth)}	NetaGrow := 0.33;
KmpA20 := 1.35; {hydrolysis rate, aerobic}	Kmp20 := 1.35;
KmpX20 := 1.35*NetaGrow; {hydrolysis rate, anoxic}	
Ksp20 := 0.027; {Ks hydrolysis}	Ksp20 := 0.027;
Kr20 := 0.032; {Ammonification}	Kr20 := 0.032;
Ka20 := 0.17; {Adsoption rate}	Ka20 := 0.17;
Kc20 := 0.04; {Conversion rate}	
{Autotrophs}	
MuHatAuto20 := 0.45; {Mu max auto}	MuHatAuto20 := 0.45;
Ksa20 := 1.0; {Ks NH4+}	Knh20 := 1.0;
Ba20 := 0.04; {B endogenous}	Ba20 := 0.04;
{PolyP Organisms}	
MuHatPolyP120 := 1.2; {Mu max - no P limit}	
KsG120 := 0.18; {Ks PHB: KsG1}	
MuHatPolyP220 := 0.42; {Mu max - P limit}	
KsG220 := 0.18; {Ks PHB: KsG2}	
Bg20 := 0.04; {B decay}	
bpp20 := 0.03; {Poly P cleavage}	
Kp20 := 6.0; {HAc uptake rate}	
{Swithes}	
Koh := 0.002; {Ks O2 Heterotrophs}	Koh := 0.002;
Koa := 0.002; {Ks O2 Autotrophs}	Koa := 0.002;
Kog := 0.002; {Ks O2 Poly P organisms}	
Kha := 0.01; {Ks NH3}	Kna := 0.01;

UCTPHO	UCTOLD
Kno := 0.1; {Ks NO3}	Kno := 0.10;
KpsH := 0.001; {Ks PO4 Heterotrophs}	
KpsP := 0.1; {Ks PO4 Heterotrophs}	
Kpp := 1.0; {Ks PO4 Poly P organisms}	
Kac := 1.0; {Ks Hac}	
{Arhenius}	
ThetaMuHatH := 1.200; {Mu max hetero}	ThetaMuHatH := 1.200;
ThetaKsh := 1.000; {Ksh hetero}	ThetaKs := 1.000;
ThetaBh := 1.029; {B endogenous hetero}	ThetaBh := 1.029;
ThetaKmpA := 1.029; {Kmp hydrolysis, aerobic}	
ThetaKmpX := 1.08; {Kmp hydrolysis, anoxic}	ThetaKmp := 1.08;
ThetaKsp := 0.910; {Ksp hydrolysis half saturation}	ThetaKsp := 0.910;
ThetaKr := 1.029; {Kr heterotrophs}	ThetaKr := 1.029;
ThetaKa := 1.029; {Ka heterotrophs}	ThetaKa := 1.029;
ThetaKc := 1.029; {Kc heterotrophic}	
ThetaMuHatA := 1.123; {Mu max autotrophs}	ThetaMuHatA := 1.123;
ThetaKsa := 1.123; {Ksa autotrophs}	ThetaKnh := 1.123;
ThetaBa := 1.029; {B endogenous autotrophs}	ThetaBa := 1.029;
ThetaMuHatP := 1.080; {Mu max Poly P organisms}	
ThetaKsG := 1.000; {KsG Poly P organisms}	
ThetaBG := 1.029; {B endogenous Poly P organisms}	
ThetaBpp := 1.029; {Bpp Poly P organisms}	
ThetaKp := 1.029; {Kp Poly P organisms}	

STOICHIOMETRIC CONSTANTS	
{Heterotrophs}	
Yzh := 0.666; {Yield}	Yh := 0.45*1.48; {Yhv = 0.45: p58} Yhv * CODVSS {0.675676}
FepH := 0.08; {fraction inert particulate}	Fe := 0.08;
fma := 1.00; {max ads/ hetero}	Fma := 1.00;
Fzbhn := 0.068; {N in biomass}	lxb := 0.1/1.48; {fn/fcv = 0.067568}
Fzehn := 0.068; {N in endogenous}	lxe := 0.1/1.48; {fn/fcv}
Fzbhp := 0.02; {P in biomass}	
Fzehp := 0.02; {P in endogenous}	
CODVSS := 1.48; {COD: VSS ratio}	CODVSS := 1.48;
{Autotrophs}	
Yza := 0.15; {Yield}	Ya := 0.15;
FepA := 0.08; {Fraction inert particulate}	
Fzban := 0.068; {N in biomass} TKNCOD/CODVSS??	
Fzean := 0.068; {N in endogenous} TKNCOD/CODVSS??	
Fzbap := 0.02; {P in biomass}	
Fzeap := 0.02; {P in endogenous}	
{PolyP Organisms}	
Yzg := 0.666; {Yield}	
FepG := 0.25; {Fraction inert particulate}	
FesG := 0.20; {Fraction inert soluble}	
FzbgN := 0.068; {N in biomass}	
FzegN := 0.068; {N in endogenous}	
Fesgn := 0.068; {N in inert soluble}	
Fzbgp := 0.02; {P in biomass}	
Fzegp := 0.02; {P in endogenous}	
Fprel := 0.5; {P rel/ HAc up}	

Fpupt := 0.75; {P up/ PHB utilised}	
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ANNEXURE C: FLOW DIAGRAM



Application for Approval of Ethics in Research (EiR) Projects
Faculty of Engineering and the Built Environment, University of Cape Town

APPLICATION FORM

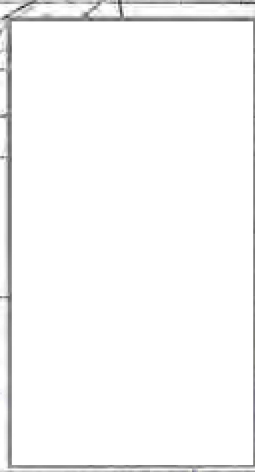
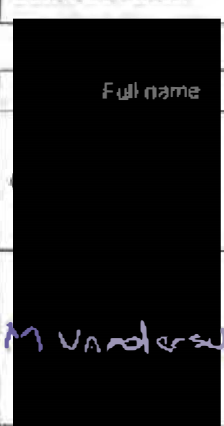
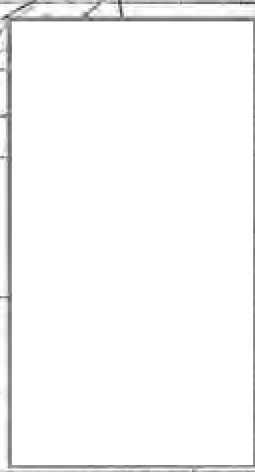
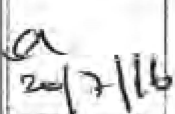
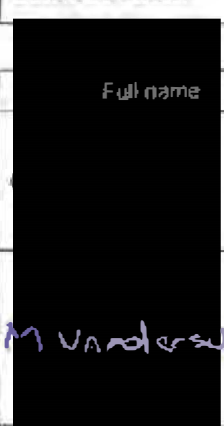
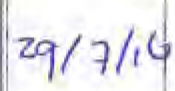
Please Note:

Any person planning to undertake research in the Faculty of Engineering and the Built Environment (EBE) at the University of Cape Town is required to complete this form **before** collecting or analysing data. The objective of submitting this application prior to embarking on research is to ensure that the highest ethical standards in research, conducted under the auspices of the EBE Faculty, are met. Please ensure that you have read, and understood the **EBE Ethics in Research Handbook** (available from the UCT EBE, Research Ethics website) prior to completing this application form: <http://www.ebe.uct.ac.za/user/aboutresearchethics.pdf>

APPLICANT'S DETAILS		
Name of principal researcher, student or external applicant	Gerard de Swardt	
Department	Civil Engineering	
Preferred email address of applicant	gerard.deswardt@mottmac.com	
If a Student	Your Degree: e.g., MSc, PhD, etc.,	MEng
	Name of Supervisor (if supervised):	Prof George Ekama
If this is a research contract, indicate the source of funding/sponsorship	n/a	
Project Title	Re-coding UCTPHD and UCTOLD in VBA	

I hereby undertake to carry out my research in such a way that:

- there is no apparent legal objection to the nature or the method of research, and
- the research will not compromise staff or students or the other responsibilities of the University;
- the stated objective will be achieved, and the findings will have a high degree of validity;
- limitations and alternative interpretations will be considered;
- the findings could be subject to peer review and publicly available; and
- I will comply with the conventions of copyright and avoid any practice that would constitute plagiarism.

SIGNED BY	Full name	Signature	Date
Principal Researcher/ Student/External applicant	Gerard de Swardt		20 Jul 2016
APPLICATION APPROVED BY			
Supervisor (where applicable)			 20/7/16
HOD (or delegated nominee) Final authority for all applicants who have answered NO to all questions in Section 1; and for all Undergraduate research (including Honours)			 29/7/16
Chair : Faculty EiR Committee For applicants other than undergraduate students who have answered YES to any of the above questions.			