DYNAMIC SIMULATION OF THE LEACHING AND ADSORPTION SECTIONS OF A GOLD PLANT

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SYNOPSIS

This dissertation describes the development of a dynamic simulator for the leaching and adsorption sections of a gold plant.

In contrast to the milling stage which precedes the leaching and which is a purely mechanical process, leaching and adsorption are hydrometallurgical processes which are of particular interest to chemical engineers. Leaching is a well defined chemical processes in which gold is dissolved out of the rock by reaction with cyanide ions. The leaching process occurs in a series of stirred tank reactors and is easily modelled.

The adsorption process is far more challenging to model. The adsorption occurs on carbon particles which are mixed into the pulp and this gives rise to the name carbon-in-pulp (CIP). The actual adsorption of the gold cyanide complex on the lattice structure of the carbon particles is a surface phenomenon which, while it has not been totally defined, can yet be described by conventional rate processes. The adsorption also takes place in a cascade of stirred tank reactors, but the occasional pumping of carbon up the cascade and the resulting counter-current movement of carbon and pulp present modelling challenges.

A dynamic simulator was regarded necessary for this process to determine what the short and long term effects of process disturbances are. While steady state models have been developed before, they are not able to describe the transient responses to such changes. Disturbances are all too common on an operating plant and as a result the plant never truly reaches a steady-state. Any control strategy for the plant must necessarily be developed by taking the transient responses into consideration. Another requirement was for the simulator to be flexible enough to be adapted quickly to various plants. It was also to be able to read in any applicable and easily available information from plant data files and to use the data to recreate reasonably accurate outputs.

The simulator is written as a collection of ordinary differential equations each of which is a mole balance of one of the components (or state variables) in the system. The mole balances include the effect of chemical reactions between the various reactants describing

the production and depletion of these components. The hydrodynamics of the bulk pulp phase are also accounted for by considering the amount of all components within process units and the movement of components between the units.

Various factors affecting the two sections of the plant have been investigated, most of which have been considered in theory or were included in simulators by earlier investigators. Some aspects, such as attrition and screen overflows, have been included in a dynamic simulator for the first time. Attrition was found to have a major effect on the efficiency of the adsorption process by levelling out the gold solution profile and thereby reducing the rate of loading on coarse carbon. Other inefficiencies are the result of unsteady operation, especially of wildly fluctuating feed flowrates which make the addition of reagents difficult to control, and various process upsets in the CIP such as screen breakages and overflows, which allow loaded carbon to move downstream with the pulp.

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NOMENCLATURE

SYMBOLS USED IN LEACH AND ADSORPTION EQUATIONS

The following section briefly explains the significance of the various symbols which are used in the equations describing the leaching and adsorption reactions.

The components of interest (gold and its derivatives) occur in three phases within the different sections of the plant and it is therefore important to distinguish which phase each component occurs in. The three phases are:

- The solid phase : the ore enters plant in its solid form and is physically reduced by milling. The gold within the ore is also solid, as are the other metals. Any concentrations of these materials or their grades are represented by G_j, where j is the particular component. G is always measured in $mol.m^{-3}$.
- The liquid phase : the ore is mixed with water. Various other reagents are dissolved in the water and react with the solid gold to bring it into solution. The concentration of any soluble component j is indicated by C_j and is also measured in $mol.m^{-3}$.
- The carbon phase is also a solid phase but is quite separate from the ore. Only certain components j are adsorbed onto the carbon and are then represented as loading terms q_j with units of mol.mol of $carbon^{-1}$.

The following symbols are used:

A = frequency factor in activation energy equation (same units as k)

A_j = exposed surface area of component j (m^2)

B = buffering constant ($.s^{-1}$)

D_j = diffusivity coefficient of component j ($m^2.s^{-1}$)

E° = activation energy as $G_j \rightarrow 0$ ($kJ.kmol^{-1}$)

f = fraction of carbon containing macropores.

G_j = grade of component j in the ore ($mol.m^{-3}$)

k = reaction rate constant (usually $.s^{-1}$, also $(kmol.m^{-3})^{-3}.s^{-1}$)

K_f = Freundlich equilibrium constant ((mol of C)$^{1/n}$.m^{-3})

K_l = Langmuir equilibrium constant (dimensionless)

K = Linear equilibrium constant (mol of C.m^{-3})

m_j = mass of component j

n = Freundlich power (dimensionless)

n_j = mols of component j

$n_{i,j}$ = mols of component j in tank i

$\dot{n}_{i,j}$ = mols of substance j leaving tank i (mol.s^{-1})

N = total number of species

NT = total number of process units in cascade

q_j = loading of component j on carbon (mol.mol of carbon^{-1})

Q_i = volume flowrate out of tank i (m^3.s^{-1})

r = radial distance from centre of carbon particle (m)

r_m = rate of reaction m (mol.s^{-1})

R = Universal Gas Constant

R_j = total radius of particles of component j (m)

$\bar{R}_j$ = average radius of particles of component j (m)

s = surface factor (dimensionless)

t = time variable (s)

T = absolute temperature (K)

$v_{i,j}$ = volume fraction of component j in tank i

V_i = volume of tank i (m^3)

V_l = volume of liquid (m^3)

w = distribution function

Greek letters:

α = constant in Brittan's (1975) rate equation

$\alpha_{j,m}$ = stoichiometric constant of species j in reaction m

δ = thickness of boundary layer (m)

μ_j = molecular mass of species j (g.mol^{-1})

ρ_j = density of component j (kg.m^{-3})

χ = ratio of the stoichiometric constants of cyanide to oxygen

Subscripts:

Au = solid gold

$Au(CN)_2^-$ = aurocyanide complex

C = carbon

Ca^{2+} = calcium ion

$Ca(OH)_2$ = calcium hydroxide

CN^- = cyanide

M = solid metal

$M(CN)_4^{3-}$ = metal cyanide complex

OH^- = hydroxide ion

f = fast leaching fraction

s = slow leaching fraction

b = in micropores

m = in macropores

p = in the pores

R = at the surface

Superscripts:

+ = concentration in equilibrium with loading

o = at t=0

eq = equilibrium at ambient conditions

∞ = at $t=\infty$

SYMBOLS USED IN INTEGRATOR EQUATIONS

a = entry in Richardson extrapolation table

with subscript s = position from right end of line

with superscript r = position from left end of line

$\underline{A}$ = vector of algebraic variables

E = Error

H = integration step size

H_{next} = estimate of next step size based on present performance

H_{pass} = step size resulting in acceptable error

i = number of integration attempts

i_{max} = maximum number of integration attempts

i_s = standard number of integration attempts

INA = index of algebraic variable vector

INX = index of state variable vector

n_i = number of sub-intervals used in the i-th integration attempt

$\underline{x} = \underline{X}$ = state variable vector

$\underline{x}_T$ = state variable vector at t = T

$\underline{x}^n$ = n-th estimate of $\underline{x}$

Greek symbols:

α = estimate of ξ

ϵ = user specified accuracy

ξ = position of the discontinuity

CHAPTER 1

INTRODUCTION

Despite the weak gold price of the past months, the importance of gold to the South African economy remains unchallenged. Towards the end of last year the Chamber of Mines of South Africa announced that the gold production for 1991 was the same as the production of the previous year at approximately 600 tons. Production was maintained despite the financially motivated closure of a few mines during the past year. The remaining producers made up for the lost output through better utilization of the available ore, by using better ore grades and (one hopes) by improving the efficiency of the extraction processes.

To ensure the competitiveness of the South African gold industry on the world market in future, further improvements will be necessary, especially in the efficiency of the extraction as the rich ores are depleted. The theory is available following a period of high activity in the research of gold extraction processes caused by the high gold price of the early eighties. The parallel development of ever more sophisticated computers during the last decade made the progression from batch experiments via steady-state simulators to dynamic simulators a natural evolution.

The system which was to be modelled was based on an existing gold plant. It consists of a leaching cascade followed by an adsorption cascade as shown in Figure 1 below.

The leach is preceded by a small aeration and buffer tank and the distributor box in which the cyanide is mixed with the pulp. The leach itself consists of ten large pachucas, which are deep continuous stirred tank reactors (CSTRs).

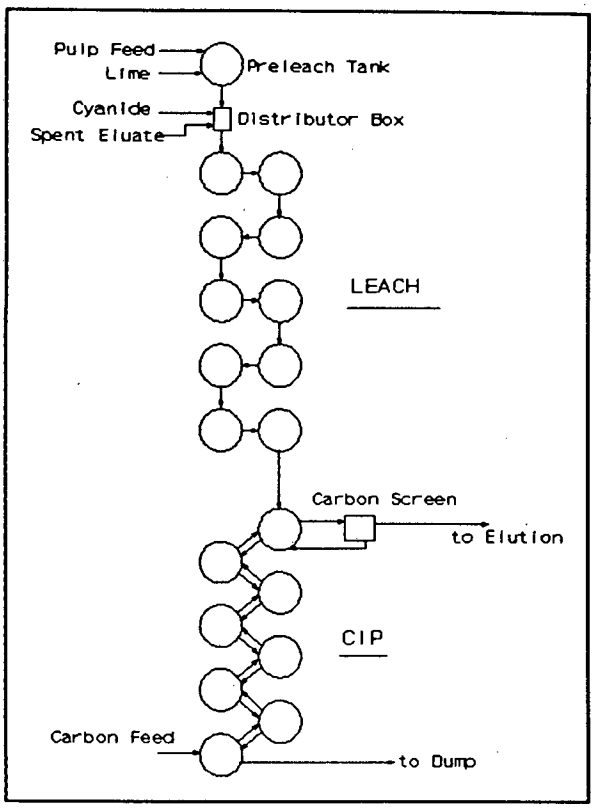


Figure 1 : Diagram of the Simulated Leach and CIP Sections

The carbon-in-pulp (CIP) section consists of eight smaller contactors. The pulp enters from the leach, flows down the cascade by gravity and then flows out to the dump. The carbon, in the form of roughly 1-2 mm diameter granules, is added at the bottom and is pumped up the cascade. It is screened from the pulp in the top-most tank and is transferred to the pre-elution tank. In the elution the gold is stripped off the carbon. The carbon is then regenerated by heating and is reused.

From the data collected on the plant by the central computer and from casual observation it was obvious that the operations never reach steady state. Partly this is the result of fluctuating amounts of ore available from the mine, varying milling characteristics and changing operation of the thickeners. What little buffering capacity is available in the pre-leach tank is not used. The overall result is a feed with constantly varying flowrate and density.

Any change in the many operating variables results in a transient response which theoreti-

cally dies away to leave the plant at a steady state. The problem on most operating plants is that the changes follow each other so quickly that the plant never leaves the period of transient response. It is precisely for this reason that a dynamic simulator is vital to study how the plant functions and how it could possibly be improved. A steady state model may be suitable for design purposes or to do an approximate mass balance over the plant, but it is simply not capable of giving enough insight on the situation within each reactor which is needed if either local loops or an overall control strategy are to be implemented. Dynamic models have the advantage over steady state ones that temporary dips in efficiency on a plant can be identified and studied.

Typically the efficiencies of both the leach and the adsorption sections are high. While the leaching reaction is relatively slow, large residence times ensure that about 95 % of the exposed gold will be dissolved. The counter-current operation of the CIP ensures even higher efficiencies, with 96-98 % of the dissolved gold usually being recovered. Yet the value of the material being treated is such that even small increases in efficiency will be financially quite rewarding. Take for instance the example of a 100 kt per month operation with a grade of 9 $g.ton^{-1}$; 97 % of the gold is available for dissolving, and of this 95 % is leached. If the efficiency of the CIP operation were increased by 0,25%, then the increase in return would be more than $ 33 000 per month.

The model was written in Fortran to comply with the Measurement and Control standard. All process equations are written in terms of mols of the different components present. Differential equations took the form of mol-balances of the pertinent species contained in each reactor, with these variables being called state variables. The total flows and individual numbers of mols leaving a tank are calculated on the basis of volume differences and are treated as algebraic variables. Flows between tanks are assumed to be instantaneous and it is also assumed that no reactions occur in the connecting streams. The integrator is a variable step method, using seconds as the time unit. A routine was specially included to track down and cross discontinuities.

The dissertation is composed of the following chapters:

Chapter 2 discusses the chemistry of leaching and adsorption by investigating how the

stoichiometry of the leaching reaction was determined, how the rate of the leaching reaction was first measured and how it was modelled. For the adsorption chemistry the nature of the activated carbon is first discussed, before a similar approach to that used in the leaching section is followed.

Chapter 3 first discusses the physical process of the plant which was modelled and then includes a section in which various simulation methods are discussed. This is followed by the detailed description of all the species included in the model, the reactions that occur between them and the rate laws by which these reactions are governed. The hydrodynamics are also discussed. Separate sections are again maintained for the two main simulated sections of the physical plant.
This chapter also describes the Numerical Integration techniques which were used and closes with a listing of all the routines as used in the actual computer program, explaining what each routine does and which part of the theory it contains.

Chapter 4 initially lists and discusses the results of the leaching section. The base case simulates the plant in its approach to steady state at constant inputs. The effect of the two main variables, the concentration of oxygen and cyanide, are investigated, followed by the effect which fluctuations in the feed flowrate and density have on the efficiency of the leach. The combined effect of badly controlled feed characteristics together with control of cyanide is outlined, while the integration of returned eluate into a control strategy of the leach completes the investigation into the leach.
The adsorption section has more variables which had to be investigated. The base case investigates the cyclic steady state which can be achieved if carbon transfers are perfectly timed and maintained at design levels. The important effect which attrition has on the efficiency is then investigated by simulating the plant without any attrition occurring. The next few subsections investigate what the effect of various different carbon transfer schemes would be. The amount of gold carried downstream by leaking carbon is simulated before the related topic of uneven carbon profiles is presented. Various plant measured variations in carbon transfer flowrate and/or starting times are shown and discussed next, followed by the effect of irregular feed flowrate. As the effect of flow irregularities often becomes visible by the blocking and overflowing of the carbon screens, the effect of such

overflows is finally also investigated.

This chapter ends with a general discussion of the major disturbances on the plant and if or how they could be controlled. Three sections are included, viz. the fluctuations in the feed to the leach and how affect the adsorption section, the possibility of controlling cyanide more effectively and finally the effect and control of carbon transfers and the carbon concentration profile.

Chapter 5 presents the conclusions of the dissertation. It summarizes the findings of the investigation and includes recommendations on the future control strategy of leaching and especially the adsorption section.

CHAPTER 2

THE CHEMISTRY OF LEACHING AND ADSORPTION

2.1 LEACHING

2.1.1 The Process

The alchemists of the eighteenth century already knew that dilute cyanide solutions were able to dissolve gold (Mellor, 1941). In 1840 A.Parkes applied for a patent for "the separation of gold or silver from their ores by digesting with a 3 to 6 per cent. soln. of cyanide of sodium, potassium, or ammonium for 3 days at 150°F to 180°F." By 1867 J.H.Rae patented the leaching of gold using cyanide and the subsequent electroplating of the dissolved gold onto copper plates and in 1885 J.W.Simpson suggested adding metallic zinc to the solution to displace the gold. (Mellor, 1941)

But it was only in 1887 that J.S.Macarthur and the brothers W. and R.W.Forrest turned cyanide leaching into an economically viable process by increasing the pH of acidic pulps to prevent the loss of cyanide, by stipulating a concentration of "8 parts of cyanogen to 1000 parts of water" and by introducing zinc powder to displace gold from solution.

2.1.2 Mechanism

In 1846 Elsner recorded that oxygen was necessary for the leaching of gold in cyanide solutions and wrote the chemical equation which is now known as Elsner's equation. In its ionic form this is :

$$4Au + 8CN^- + O_2 + 2H_2O \rightarrow 4Au(CN)_2^- + 4OH^- \quad \ldots\ldots\ldots \quad \text{(L-1)}$$

At the end of the same century, Bodländer published his ideas on the chemistry of

leaching. He proposed a two step process :

$$2Au + 4CN^- + O_2 + 2H_2O \rightharpoonup 2Au(CN)_2^- + 2OH^- + H_2O_2 \quad \ldots\ldots \text{(L-2a)}$$

$$2Au + 4CN^- + H_2O_2 \rightharpoonup 2Au(CN)_2^- + 2OH^- \quad \ldots\ldots\ldots \text{(L-2b)}$$

Added together these two equations are the same as Elsner's equation, but with the important difference, that the presence of H_2O_2, which Bodländer had detected in the solution, could be explained.

Barsky et.al.(1934), showed that the equilibrium constants of all three reactions were large and positive, indicating that thermodynamically the products are stable and the reaction should proceed as written. Which mechanism is actually the most important remained a point of contention for a long time, especially as various authors disputed the presence of the H_2O_2 intermediate (Deitz and Halpern, 1953; Kudryk and Kellogg, 1954).

Kudryk and Kellogg (1954) postulated that the leaching process was essentially equivalent to corrosion, with the anodic and cathodic reaction halves occurring in adjacent regions on the gold surface. The anodic reaction in Elsner's and both Bodländer's equations is the same:

$$Au + 2CN^- \rightharpoonup Au(CN)_2^- + e^- \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(L-3)}$$

The differences lie in the cathodic reactions:

In (L-1): $H_2O + \frac{1}{2}O_2 + 2e^- \rightarrow 2OH^-$ $\ldots\ldots\ldots\ldots\ldots\ldots\ldots$ (L-4)

In (L-2a): $2H_2O + O_2 + 2e^- \rightarrow 2OH^- + H_2O_2$ $\ldots\ldots\ldots\ldots\ldots\ldots$ (L-5)

In (L-2b): $H_2O_2 + 2e^- \rightarrow 2OH^-$ $\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$ (L-6)

Figure 2, taken from Kudryk and Kellogg, shows these interacting cells diagrammatically. They assumed that equation L-4 represents the cathodic reaction.

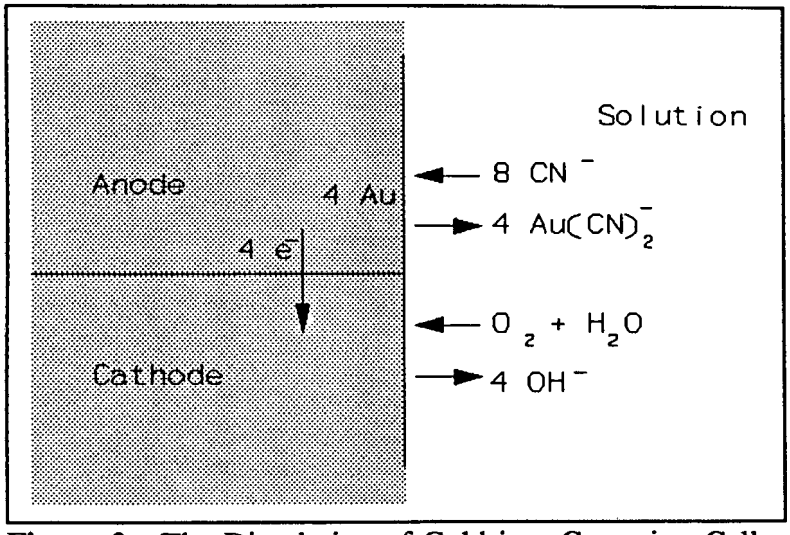


Figure 2 : The Dissolution of Gold in a Corrosion Cell

Increased levels of both oxygen (White, 1934; Fahrenwald and Newton, 1939) and peroxide (Mellor, 1941) in water were found to increase the rate of leaching, but at high concentrations, both were found to passivate the surface (Cathro and Koch, 1963a,b; Cathro, 1963). Recently additions of both oxygen and peroxide have again been suggested to improve leach-efficiencies: oxygen - Arnold and Stephens (1988), Rodrigues (1990); peroxide - Lorösch et.al.(1988), Lorösch (1990), Osthof (1990).

Various authors reported that as the cyanide concentration in the solution increases, a change-over occurs from the diffusion-control by cyanide to that of oxygen. If Elsner's equation described the process fully, this change-over should occur approximately at $\frac{C_{CN^-} D_{CN^-}}{C_{O_2} D_{O_2}} = 8$ where C_{CN^-} and C_{O2} are the bulk concentrations of free cyanide and dissolved oxygen in solution respectively and D_{CN^-} and D_{O2} are their diffusivities, while If, on the other hand, Bodländer's first equation is applicable (as suggested by Kameda, 1949) the change-over should occur at $\frac{[CN^-]D_{CN^-}}{[O_2]D_{O_2}} = 4$.

Again investigators were divided into the group supporting the first (Kudryk and Kellogg, 1954) and those supporting the second (Deitz and Halpern, 1953; Kakovskii and Kholmanskikh, 1960; Habashi, 1966).

Finkelstein (1972) showed that 85% of the H_2O_2 produced in Bodländer's first equation diffuses away, while part of the remaining 15% undergoes auto-oxidation to O_2 and H_2O and only the remaining portion takes part in the second reaction.

2.1.3 General Chemistry of Gold, its Ions and Complexes

Gold, Silver and Copper are among the most noble metals. They occur in the earth's surface in their metallic form in pockets of relatively high concentrations, so that they were discovered early in human history and were the first metals that were mined and used (Dickerson et.al.,1984). The nobility of these metals is the effect of their valence electron configuration (or aufbau): essentially their outer d-orbitals should be filled with the exception of one place. But as a completely filled d-orbital has a lower energy, one electron from the next s-orbital is used to fill the d-orbital completely. This gives the metal a highly stable state. Gold has the following aufbau:

Au(0) : Xe $4f^{14}$ $5d^{10}$ $6s^{1}$

where Xe refers to the aufbau of the previous noble gas xenon.

When gold is involved in chemical reactions, it will usually form either the Au(I) or the Au(III) states, with the Au(II) and Au(IV) states being much less common.The electron configurations of the two more common gold ions are:

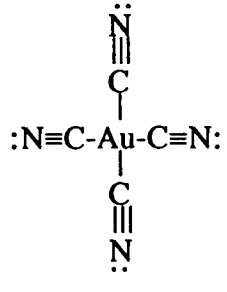
Au(I) : Xe $4f^{14}$ $5d^{10}$ $6s^{0}$

Au(III) : Xe $4f^{14}$ $5d^{8}$ $6s^{0}$

In the reaction with cyanide two gold complexes are possible: the aurous cyanide complex ($Au(CN)_2^-$) and the auric cyanide complex ($Au(CN)_4^-$). Their respective aufbaus are:

Au(I) in :N≡C-Au-C≡N: : Xe $4f^{14}$ $5d^{10}$ $6s^{2}$ $6p^{2}$

Au(III) in : Xe $4f^{14}$ $5d^{10}$ $6s^{2}$ $6p^{4}$ (Wells, 1962)



Both complexes are very stable. The gold atom in the first complex involves two sp-hybridized orbitals forming a linear molecule which has a stability constant of 2.10^{38} (Finkelstein, 1972). The second involves bonds of four dsp^2-hybridized orbitals, giving a square planar shape (Wells, 1962) to the molecule which is even more stable as shown by its stability constant of 10^{56}. In both cases the 6s orbital is filled, while the 6p orbital is only partly filled. The great stability of both complexes lies in the filling of the 6s orbitals which shields all lower orbitals and in the covalent bonds between the gold and carbon atoms.

The effectiveness of cyanide in leaching noble metals like gold and silver lies in its provision of reaction paths at lower potentials. The standard reduction potentials of the two gold-ion producing reactions are shown below. These indicate that under normal circumstances (ie. in the absence of cyanide but in the presence of a strong oxidant), the auric ion has a lower reduction potential and would therefore be more likely to form than the aurous ion.

$$Au^{+} + e^{-} \rightarrow Au \ , \ E^{\circ} = 1{,}68V \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad \text{(L-7)}$$

$$Au^{3+} + 3e^{-} \rightarrow Au \ , \ E^{\circ} = 1{,}50V \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad \text{(L-8)}$$

Both the aurous and auric ions are stronger oxidants than water and would therefore, if added to the system be reduced to metal gold by oxidizing water to oxygen (in the opposite reaction to the one in equation L-9 below):

$$4H^{+} + O_2 + 4e^{-} \rightarrow 2H_2O \ , \ E^{\circ} = 1{,}228V \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad \text{(L-9)}$$

In the case where cyanide is added to the system, though, a different picture emerges. The standard reduction potential of the reaction of $Au(CN)_2^-$/Au reaction is shown below:

$$Au(CN)_2^- + e^{-} \rightarrow Au + 2CN^{-} \ , \ E^{\circ} = 0{,}50V \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad \text{(L-10)}$$

The effect of this couple is shown on the Pourbaix Diagram (adapted from Finkelstein, 1972) of the Gold-Water-Cyanide system in Figure 3: The potential of the reaction shown in equation L-10 lies below that of the H_2O/O_2 pair and thus metallic gold will be oxidised to aurocyanide in the presence of cyanide.

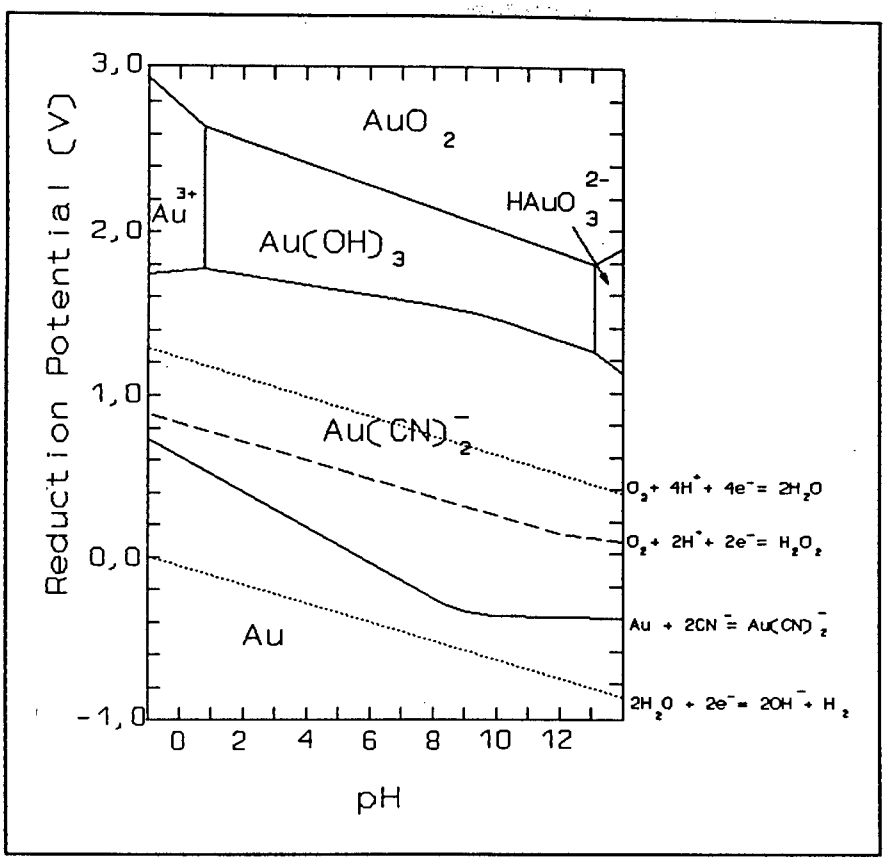


Figure 3 : Pourbaix Diagram of the Au-CN^--H_2O System at 25°C. Concentration of all dissolved substances = 10^{-4} mol.l^{-1}. Partial pressures of H_2 and O_2 = 1 atm.

2.1.4 Rate Equation

Already the first researchers to study the leaching of gold by cyanide noticed that the rate of gold dissolution increased with increasing concentrations of cyanide and oxygen (White, 1934; Fahrenwald and Newton, 1939). Fink and Putnam (1950) found other factors which affected the rate: sulphides retarded the rate, while traces of lead, bismuth, mercury and thallium salts were found to accelerate it. As explained by Cathro (1963) the base metal salts prevent passivation. Habashi (1970) mentions the coating effect of CaO_2 from the oxidation of lime.

Kameda (1949) was the first to publish a rate equation to describe the leaching of gold. It models the diffusion of cyanide to the gold surface through a stagnant layer using Fick's law:

$$r_{Au} = \frac{D_{CN^-} A_{Au}}{\delta} \left(C^{o}_{CN^-} - C_{Au} \right) \quad \text{(L-11)}$$

where r_{Au} is the rate of gold dissolving,

A_{Au} is the exposed surface of gold,

δ is the thickness of the boundary layer and

$C^{o}_{CN^-}$ is the bulk concentration of free cyanide at t=0.

Essentially this assumes that one cyanide ion needs to diffuse to the gold surface to leach each gold atom. Obviously that is incorrect and is especially surprising, as Kameda knew the stoichiometries of Elsner's equation as well as both of Bodländer's equations.

The diffusion of the reactants was also the basis of the model proposed by Kudryk and Kellogg (1954). They used the stoichiometry of the leaching reaction according to Elsner. The rate of gold dissolution is predicted to be half that of cyanide consumption and four times that of oxygen consumption. So depending on which is rate-determining, either of the following equations must be used:

$$r_{Au} = \frac{r_{CN^-}}{2} = \frac{D_{CN^-}}{2\delta} \left(C_{CN^-} - C_{CN^-,R} \right) \quad \text{(L-12a)}$$

$$r_{Au} = 4 r_{O_2} = \frac{4 D_{O_2}}{\delta} \left(C_{O_2} - C_{O_2,R} \right) \quad \text{(L-12b)}$$

where r_{CN^-} and r_{O_2} are the rates of cyanide and oxygen consumption, respectively, and $C_{CN^-,R}$ and $C_{O2,R}$ are the concentrations of cyanide and oxygen at the surface of the gold particle.

Habashi (1966) had the same approach, but used Bodländer's first equation. He built the change-over from diffusion-control by cyanide to diffusion-control by oxygen into his equation:

$$r_{Au} = \frac{2 A_{Au} D_{CN^-} D_{O_2} C_{CN^-} C_{O_2}}{\delta \left\{ D_{CN^-} C_{CN^-} + 4 D_{O_2} C_{O_2} \right\}} \quad \text{(L-13)}$$

Loveday et.al.(1970) used a distribution of zero-order rate constants as they proposed that the reaction was rate-limiting rather than the diffusion of reactants to the gold surface. Their rate equation is:

$$r_{Au} = \int_0^{\infty} k w(k,0) dk \qquad \text{(L-14)}$$

For w(k,0) they used the Schumann distribution.

Brittan and van Vuuren (1973) proposed a fairly complex model taking into account many variables which had been recorded on daily log-sheets of various mines. These variables included the temperature, pH and cyanide concentrations in the first and last leach pachucas. Various densities and size group percentages were also included.

Brittan (1975) then published a rate equation which essentially lumps all rate-controlling effects into an Activation Energy term, which changes with changing concentration of gold in the ore:

$$r_{Au} = A \exp\left[\frac{-E^{\circ}}{RT}(1 - \alpha G_{Au})\right] \qquad \text{(L-15)}$$

where α is a constant and

G_{Au} is the grade of gold in the ore.

2.2 ADSORPTION ON CARBON : CARBON-IN-PULP

2.2.1 The History of Carbon in Gold Extraction

The absorptive powers of charcoal have been known for centuries. McDougall (1991) reports that it was already used as a clarifying agent in the Egyptian civilization and Bailey (1987) reported that the ancient Hindus used activated carbon to clarify water. The use of carbon was developed further throughout the centuries to absorb colours, odours and poisons from various media.

By the 1880s carbon was added to clarified chloride-leach liquors to 'precipitate' the gold. The carbon was subsequently burned to release the gold. A similar process was patented in 1894 after the cyanidation-route became common for gold leaching, in which the gold-cyanide was precipitated using carbon (Laxen et al,1979). Despite the cost of the carbon, which could obviously be used only once, a few plants continued to use carbon precipitation into this century. Most plants rather chose filtration followed by either zinc-precipitation or electroplating instead.

It was only in the fifties of the present century that Zadra at the U.S.Bureau of Mines, at the request of the Getchell Mine in Nevada (Laxen et.al., 1979), investigated the possibility of stripping the gold off the carbon by chemical means rather than burning it. The first patent used sodium sulphide (Zadra, 1950) but because the proposed process was not able to retrieve the adsorbed silver, another process was developed using sodium hydroxide together with cyanide (Zadra, 1952). The solution was circulated through an elution column containing the loaded carbon and an electroplating chamber which stripped the solution of its gold content.

The first application of this new technology was at Carlton Mill, Cripple Creek, Colorado in 1961 (Laxen et.al.,1979), where it was used to retrieve gold from slimes. The next milestone was reached when a large carbon-in-pulp (CIP) plant was put into operation at the Homestake Mine, South Dakota in 1973 (Sisselman, 1976).

In 1974 Davidson developed a new process (now called the AARL process) for the elution of gold from carbon. Instead of recycling the eluate through the elution column and the electroplating chamber, he initially pretreated the carbon with a carbonate solution and then washed the carbon with hot deionized water (Davidson, 1974). The solution was then stripped of its gold in batches before being pumped to the leach. An improvement was suggested by Davidson and Duncanson (1977) which used a strong cyanide solution during the pre-treatment instead.

While the first CIP plant to be commissioned in South Africa in 1978 was fairly small - treating 10 000 t/m at Modderfontein 74 - by 1980 two larger plants were already operational, and by 1985 the total had risen to 17 (Bailey, 1987). Davidson and Schoeman (1991) estimated the present number of CIP operations in South Africa at about 60.

2.2.2 Activated Carbon

Activated carbon has the ability to absorb large amounts of various substances from aqueous solutions. This is caused by the structure of carbon within the particles of activated carbon.

The activation of carbon involves taking some organic material, such as peach pips, wood or, as is usual today, coconut shell, and heating it to high temperatures in a controlled atmosphere. All volatile constituents within the organic material are gasified, leaving only the carbon backbone behind. Part of the carbon reacts with oxygen in the air so that pores are burnt into the carbon. The pores are divided into groups according to their sizes. Cho et.al.(1979a) divided them into three size groups: macropores, transitional pores and micropores. The exact sizes of these pores obviously depend on the size definition used. McDougall (1991) categorizes pores as shown in Table I.

The percentages of total area that the different pore sizes contribute depends on the type of raw material used and clearly also on the definition of the pore sizes and the associated method of measuring them (eg. see Peel et.al.(1981) and Cho and Pitt (1983) for different definitions). The percentages quoted above refer to coconut carbon, which produces an

unusually large number of micropores. The large surface area associated with the micropores, which is available for adsorption of gold makes this the favourite carbon in CIP plants today.

Pore Types	Size Range (in Å)	% of Surface Area
Macropores	500-20000	~0%
Mesopores	100-500	5%
Micropores	8-100	95%

Table I : Pore Definitions

The structure of the Carbon backbone is very similar to graphite. It consists of little graphite platelets (Cho and Pitt,1983) a few atoms thick and 20 - 100 Å in diameter, which are randomly stacked on one another giving a 'turbostatic' structure (McDougall, 1991). The edges of these platelets stick out into the pores and the unsatisfied bonds of the surface atoms result in reactive sites (Cho and Pitt, 1979a).

The nature of these active sites has been the topic of many discussions as the type of site would determine the type of adsorption process that would be most likely to occur on it. This is discussed below.

2.2.3 Mechanism

Various mechanisms have in the past been suggested for the form in which the gold is adsorbed on the surface of the carbon and have been discussed at length by various authors (eg. McDougall et.al.,1980; Bailey,1987; Adams et.al.,1987). Essentially they can be grouped into the following mechanisms:

- reduction of $Au(CN)_2^-$ to metallic gold,
- loss of CN^- from $Au(CN)_2^-$ to give either
    - AuCN, or
    - neutral macromolecules with the general formula $Au_n^+(CN^-)_n$, (Jones et.al.,1988)

- oxidation of the gold atom in $Au(CN)_2^-$ to give $Au^{n+}(CN^-)_n$,
- adsorption of ions in an electrical multilayer,
- specific adsorption of ion pairs $[M^{n+}][Au(CN)_2^-]_n$, where M is a metal, eg.Ca,Na,K
- non-specific adsorption of ions on the carbon surface.

In the normal conditions of an adsorption circuit (high pH, high $[CN^-]$, low temperatures) the reduction of $Au(CN)_2^-$ is unlikely (Tsuchida et.al., 1984). This is supported by Jones et.al. (1989) who found that the adsorption of $Au(CN)_2^-$ is thermodynamically reversible even in the absence of CN^-, which would not be possible if adsorption was accompanied by a loss of cyanide from the complex. Adams et.al.(1987b) found that the formation of AuCN may occur at low pH or at high temperatures, such as in the pre-elution acid-wash or during regeneration.

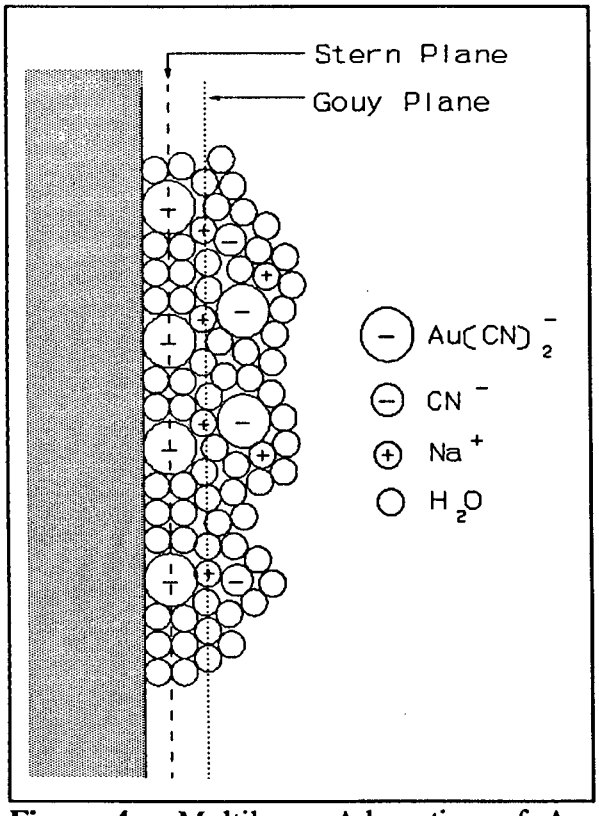


Figure 4 : Multilayer Adsorption of $Au(CN)_2^-$ and Other Ions

The mechanism postulated by Cho and Pitt (1979b) describes the adsorption of the $Au(CN)_2^-$ ion on active sites on the carbon, balanced by positive ions which adsorb non-specifically in a multilayer of positive metal ions and more negative ions including CN^-

and $Au(CN)_2^-$ (refer to Figure 4 for a schematic representation, taken from Cho and Pitt). Their use of Solvation Theory explained why the larger $Au(CN)_2^-$ molecules adsorbed more readily than the smaller $Ag(CN)_2^-$ molecules or the more negatively charged $Cu(CN)_4^{3-}$.

While Adams et.al.(1987b) agreed that activated carbon has a greater affinity for larger and less charged molecules, they discounted the multilayer type of adsorption because it could not explain why ClO_4^- doesn't load as well as $Au(CN)_2^-$. They suggested that loading was rather due to adsorption of ion pairs on certain active sites.

Jones et.al.(1989) found that the two -C≡N bonds were perfectly symmetrical. As the two nitrogen atoms are slightly negative with respect to the gold atom $\overset{\delta-}{:N}\equiv\overset{\delta+}{C}:Au:\overset{\delta-}{C}\equiv N:$, any interaction with a cation would have to occur at the nitrogen atoms. The formation of a definite ion pair implies that only one cation is involved and this cation could only have interacted with one of the two nitrogen atoms. Such one-sided interaction would have caused the molecule to become asymmetric but as this is contrary to observation, the formation of definite ion pairs can be discounted.

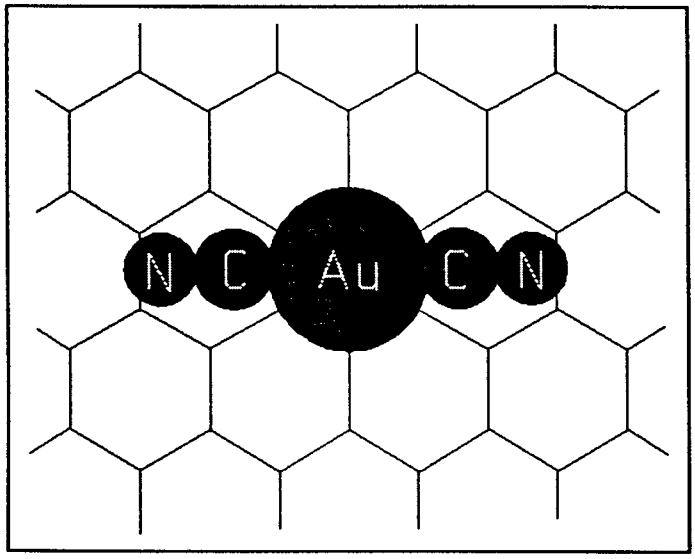


Figure 5 : $Au(CN)_2^-$ Adsorbed on Graphite

Instead, the $Au(CN)_2^-$ ion is "adsorbed in a linear state parallel to the graphitic planes of the carbon. The adsorption bond is formed by charge donation (0.3 - 0.5e$^-$) to the central

gold cation from the delocalised π-electron system of graphite" (quoted from Jones et.al.,1988). Jones et.al showed diagrammatically how well $(NC\text{-}Au\text{-}CN)^-$ fits onto the carbon backbone. Their diagram is reproduced in Figure 5. The positive metal ions adsorb non-specifically onto the carbon with the charge being balanced by the delocalised electron cloud. McDougall (1991) suggests that the main function of the various surface groups which were reported to be present on activated carbon (Tsuchida et.al.,1984; Adams et.al.,1987; Adams, 1989), is to make the essentially hydrophobic carbon more hydrophillic, rather than functioning as adsorption sites.

2.2.4 Factors Affecting Adsorption

From the first articles published on CIP, factors which affect the rate of loading and the equilibrium loading have been discussed.

Factors influencing the rate are :

- carbon particle size (Dixon et.al.,1978; Davidson et.al.,1979; Fleming and Nicol, 1984)
- ionic strength (Davidson, 1974; Cho and Pitt, 1979b)
- type of cations in solution (Davidson, 1974; McDougall et.al.,1980; Davidson et.al., 1982; Tsuchida et.al.,1984)
- temperature (Davidson, 1974; Dixon et.al.,1978; Cho et.al.,1979b; McDougall et.al.,1982; Davidson et.al.,1982; Splaine et.al.,1982)
- pH (Davidson, 1974; Davidson et.al.1979; Davidson et.al.,1982; Bailey, 1987)
- stirring (Fleming and Nicol, 1984; Hughes and Linge, 1989)
- dissolved oxygen concentration (v.d.Merwe and v.Deventer, 1988)
- ore particles (Jones and Linge, 1989; Jordi et.al.,1991)
- pulp density (Fleming and Nicol, 1984)

Factors affecting the equilibrium loading are :

- competing species (Davidson et.al.,1982; Fleming and Nicol,1984; Tsuchida et.al.,1984; Adams et.al.,1987b). The competing species in order of their loadabilities are:

  $Hg(CN)_2 > Ag(CN)_2^- > Cu(CN)_2^- > Cu(CN)_3^{2-} > Ni(CN)_4^{2-} > Cu(CN)_4^{3-} >$

$Co(CN)_6^{3-} > Fe(CN)_6^{3-}$

- carbon type and preparation (Menne, 1982; Cho and Pitt, 1983)
- temperature (Splaine et.al.,1982)
- pH (Dixon et.al.,1978; Cho and Pitt,1979b; Davidson et.al.,1979; Davidson, 1986)
- dissolved oxygen (v.d.Merwe and v.Deventer, 1988)
- ionic strength (Fleming and Nicol, 1984)
- calcium carbonate scale (Davidson, 1986; Mattioli et.al.,1990)
- other inorganic foulants (La Brooy et.al., 1986; Jones et.al.,1988b)
- organic foulants (Fleming and Nicol, 1984; La Brooy et.al., 1986)

Good summaries of these effects are give by Fleming and Nicol (1984), Johns (1987) and Vetter (1987).

The efficiency of any adsorption circuit will also be affected by other factors, such as the loss of carbon from the circuits by degradation or leakage through the intermediate screens (Sorensen, 1989; Whyte et.al., 1990) or the loss of cyanide from the circuit through side reactions which are catalyzed by the activated carbon (Muir et.al.,1988; Adams 1990 a,b).

2.2.5 Rate Equations

Quite a number of possible rate expressions have been suggested for the adsorption of aurocyanide onto activated carbon (Woollacott et.al.1990). It is usual to divide the models into empirical and mechanistic ones.

The first empirical models were not in the form of differential equations, but rather incorporated time into the expression:

Fleming et.al.(1980): $q_{Au(CN)_2^-} = k C^{o}_{Au(CN)_2^-} t^{n}$ . . . . . (C-1)

where $q_{Au(CN)_2^-}$ is the loading of aurocyanide on carbon,

$C^{\circ}_{Au(CN)_2^-}$ is the bulk solution concentration at t=0 of aurocyanide and

n is a constant

La Brooy et.al.(1986): $q = k C_{Au(CN)_2^-} t^n$ ..... (C-2)

where $C_{Au(CN)2^-}$ is the bulk solution concentration of aurocyanide

These are obviously useless for dynamic simulations. Later investigators used the film diffusion model instead:

$$r_{Au(CN)_2^-} = k\left(C_{Au(CN)_2^-} - C^{+}_{Au(CN)_2^-}\right) \quad \text{..... (C-3)}$$

where $C^{+}_{Au(CN)2^-}$ is the concentration of aurocyanide in solution which is in equilibrium with the loading of aurocyanide on carbon $q_{Au(CN)2^-}$. Some relationship between $C^{+}_{Au(CN)2^-}$ and $q_{Au(CN)2^-}$ must be substituted into the equation (Woollacott et.al., 1990), such as

- a linear relationship as used by Nicol et.al.(1984) :

$$r_{Au(CN)_2^-} = k\left(C_{Au(CN)_2^-} - K\, q_{Au(CN)_2^-}\right) \quad \text{..... (C-4)}$$

- a Freundlich isotherm as used by Johns (1986) :

$$r_{Au(CN)_2^-} = k\left[C_{Au(CN)_2^-} - \left(\frac{q_{Au(CN)_2^-}}{K_f}\right)^{\frac{1}{b}}\right] \quad \text{..... (C-5)}$$

where b is a constant and

K_f is the Freundlich equilibrium constant

- a Langmuir isotherm suggested in this form by Woollacott et.al.(1990) :

$$r_{Au(CN)_2^-} = k\left[C_{Au(CN)_2^-} - \frac{K_l q_{Au(CN)_2^-}}{q^{\infty}_{Au(CN)_2^-} - q_{Au(CN)_2^-}}\right] \quad \text{..... (C-6)}$$

where K_l is the Langmuir equilibrium isotherm, and

$q^{\infty}_{Au(CN)2^-}$ is the loading capacity of aurocyanide on the particular carbon.

At low loadings, each of these equations may be reduced to

$$r_{Au(CN)_2^-} = k C_{Au(CN)_2^-} \quad \text{..... (C-7)}$$

If the loading is far from equilibrium, so that ($q^{\infty}_{Au(CN)2^-}$ - $q_{Au(CN)2^-}$) does not vary significantly, equation (C-6) reduces to the more familiar equation used by Dixon et.al.(1978):

$$r_{Au(CN)_2^-} = k'\left[C_{Au(CN)_2^-}\left(q^{\infty}_{Au(CN)_2^-} - q_{Au(CN)_2^-}\right) - K_l q_{Au(CN)_2^-}\right] \quad \text{..... (C-8)}$$

The film diffusion model assumes that the rate limiting step lies in the diffusion of the aurocyanide ion from bulk solution to the carbon surface. That is not necessarily correct. As Peel et.al.(1981) note, there are four steps involved in the transport of the ion from the solution to the surface of the micropore:

i) first it diffuses through the boundary layer to the carbon surface,

ii) then it must adsorb onto the outside surface,

iii) diffuse along the macropore surface and

iv) from there diffuse into the micropore.

A mechanistic model will try to take into account which ever of these are needed to describe the process more closely (le Roux, 1991).

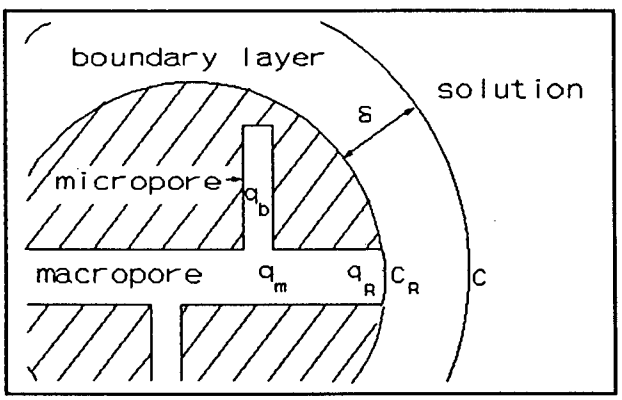


Figure 6 : Schematic of Carbon Particle

Peel et.al.(1981) describe their system with the following equations (see Figure 6 for a schematic of the carbon particle showing the various concentration and loading terms):

film diffusion to particle surface:

$$\frac{dC_{Au(CN)_2^-}}{dt} = -k\left(C_{Au(CN)_2^-} - C_{Au(CN)_2^-,R}\right) \quad \text{. . . . . (C-9)}$$

equilibrium at the particle surface:

$$k\left(C_{Au(CN)_2^-} - C_{Au(CN)_2^-,R}\right) = \frac{fD_{Au(CN)_2^-,R}\,C_c}{r_c}\left.\frac{\partial q_{Au(CN)_2^-,m}}{\partial r}\right|_R \quad \text{. . . . . (C-10)}$$

surface diffusion in macropore:

$$f\frac{\partial q_{Au(CN)_2^-,m}}{\partial t} = \frac{fD_{Au(CN)_2^-,R}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial q_{Au(CN)_2^-,m}}{\partial r}\right) - r_{Au(CN)_2^-,b} \quad \text{. . . . . (C-11)}$$

diffusion into micropore:

$$r_{Au(CN)_2^-,b} = (1-f)\frac{\partial q_{Au(CN)_2^-,b}}{\partial t} = k_b\left(q_{Au(CN)_2^-,m} - q_{Au(CN)_2^-,b}\right) \quad \ldots\ldots\ldots \text{(C-12)}$$

together with the necessary Initial and Boundary Conditions.

$q_{Au(CN)2^-,m}$ is the loading of aurocyanide in the macropore

$q_{Au(CN)2^-,b}$ is the loading of aurocyanide in the micropore

$C_{Au(CN)2^-,R}$ is the solution concentration of aurocyanide at the particle surface

$D_{Au(CN)2^-,R}$ is the diffusivity of aurocyanide at the particle surface

C_c is the concentration of carbon in the tank

The macropore diffusion equation is simply the equation of continuity for constant density and diffusivity in spherical coordinates with the assumption that diffusion occurs only in a radial direction (Bird et.al.,1960) and was first suggested for aurocyanide adsorption by Cho and Pitt (1979a). The carbon has been subdivided into the fraction containing macropores, f, and the remaining fraction containing micropores, (1-f).

Peel et.al.(1981) used the Freundlich isotherm to describe the relationship between the solution concentration at the interface $C_{Au(CN)2^-,R}$ and the loading at the interface $q_{Au(CN)2^-,R}$:

$$q_{Au(CN)_2^-,R} = \left(\frac{C_{Au(CN)_2^-,R}}{K_f}\right)^n$$

van Deventer (1984a) defines the Freundlich isotherm in terms of the bulk solution $C_{Au(CN)2}$ which is related to the loading at the interface:

$$q_{Au(CN)_2^-,R} = q_{Au(CN)_2^-,m}(R,t) = \left(\frac{C_{Au(CN)_2^-}}{K_f}\right)^n$$

Used as a boundary condition, this makes the linear film diffusion gradient in (C-9) and (C-10) redundant. On eliminating the diffusion gradient from these equations we get:

$$\frac{dC_{Au(CN)_2^-}}{dt} = \frac{-fD_{Au(CN)_2^-,R}C_c}{r_c}\left.\frac{\partial q_{Au(CN)_2^-,m}}{\partial r}\right|_R \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(C-13)}$$

In his later papers van Deventer (1984b and 1986b) replaces the radial diffusion term

$r^2 \frac{\partial q_{Au(CN)_2^-,m}}{\partial r}$ by a quadratic approximation $\frac{(q_{Au(CN)_2^-,R})^2 - (q_{Au(CN)_2^-,m})^2}{2q_{Au(CN)_2^-,m}}$. This automatically removes the dependence of macropore loading on radial distance, reducing the $q_{Au(CN)2^-,m}(r,t)$ to the average loading $\overline{q}_{Au(CN)2^-,m}(t)$ and also reducing the partial derivatives with respect to time to simple derivatives. An extension is made to a multicomponent system (van Deventer, 1986c) which uses the Sheindorf multicomponent isotherm. In that particular paper, van Deventer uses this to model a two-component system.

Brinkmann and King (1987) used a slightly different approach to that suggested by Peel et.al. in that they simply assume that the concentration of aurocyanide at the mouth of the macropore is the same as the concentration in the bulk solution, $C_{Au(CN)2^-}$, (i.e. no film diffusion). The aurocyanide complex then diffuses along the macropore and adsorbs only once it reaches the micropores. The equations are similar to those of Peel et.al.(1981) except that $q_{Au(CN)2^-,m}$ has to be replaced by $C_{Au(CN)2^-,p}$ (the concentration of aurocyanide in the solution within the pore) and $q_{Au(CN)2^-,b}$ essentially signifies the adsorbed species.

2.3 CONCLUDING REMARKS

The amount of knowledge on gold leaching and adsorption has grown rapidly during the last century. For the largest part of this period most researchers were involved with explaining how leaching works and how it can be modelled.

With the sharp rise of the gold price in the early 1980's and the introduction of the CIP processes on South African plants, most researchers' attentions shifted to the adsorption process. Intensive investigation started into the fundamentals of the loading process and the factors affecting it. As a result the amount of information available in this area of research is unusually large, despite the short period of investigation.

Dynamic simulators of the CIP process appeared in the second half of the 1980's and the interest in this application continues into the present decade as the use of these simulators for better process and control design of the adsorption section becomes a necessity.

CHAPTER 3

THE SIMULATOR

The aim of this project was to write a dynamic model to simulate the leach and adsorption sections of a gold plant. The simulator was to be able to read in data collected on a running plant and to use these to make predictions of the amount of gold leached, adsorbed and lost. It was also to be flexible enough for efficiency studies to be conducted on it.

3.1 SIMULATED PROCESS

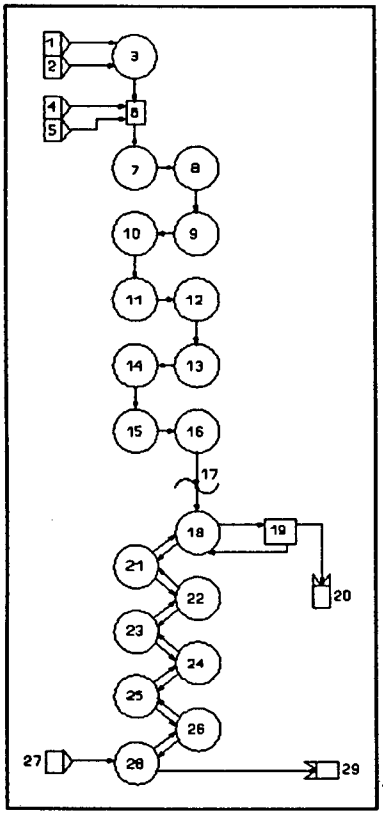


Figure 7 : The Simulated Plant Units

Key :

Unit No.	Description
1	Pulp Feed Unit
2	Lime Addition Unit
3	Pre-leach Tank
4	Cyanide Addition Unit
5	Spent Eluate Addition Unit
6	Distributor Box
7-16	Leach Pachucas
17	Magic Box
18	First CIP Tank
19	Carbon Screen
20	Loaded Carbon Sink
21-26	CIP Tanks
27	Fresh Carbon Feed
28	Last CIP Tank
29	Discard Pulp Sink

The data used in the simulator was collected at a South African gold plant on an earlier Mintek project over a period of two years. The configuration of that plant was therefore also used and is shown diagrammatically in Figure 7. It is similar to Figure 1 but in Figure 7 the units are numbered as they are referred to in the simulation program and the feed units and sink units (the need for which is described in section 3.2) are included.

The part of the plant which was simulated consists of:

- The pre-leach tank, into which the exit stream from the thickeners is pumped after being screened. The pulp is air-agitated to keep it well mixed. Any extra lime needed to correct the pH in the leach is added here.
- The distributor box, in which the leach feed pulp is mixed with cyanide and the eluate which is returned from the smelt house,
- The leach cascade consisting of ten large pachucas. Each pachuca is agitated by a large mechanical stirrer inside a downdraught tube as shown in Figure 8. This ensures good mixing and minimizes short-circuiting of the pulp. Compressed air is added in the downdraught tubes so that it is carried to the bottom of the tank by the pulp. This gives the air maximum contact time with the pulp which ensures that dissolved oxygen levels are high throughout the cascade.

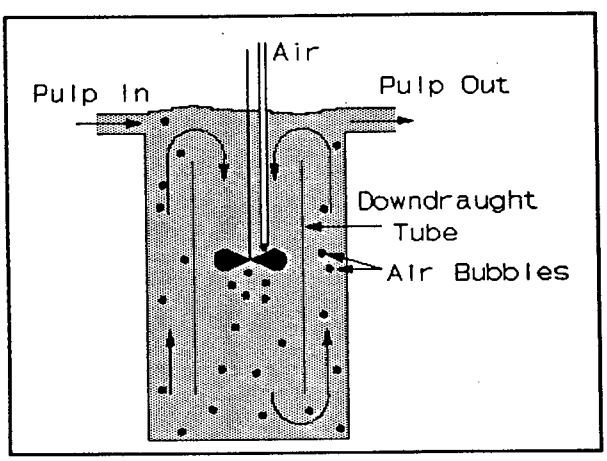


Figure 8 : Leach Pachuca

- The carbon-in-pulp section consisting of eight small contactors which are shown in Figure 9. The pulp is mechanically agitated, but no air is added. The carbon is retained in the contactors by horizontal screens while the pulp is forced through by its own hydrostatic pressure. The pulp flows down the cascade under the force

of gravity while carbon-containing pulp is periodically pumped up the cascade. A mixture of reactivated and fresh carbon is added to the bottom-most contactor, while the carbon is screened out of the pulp originating in the top-most tank.

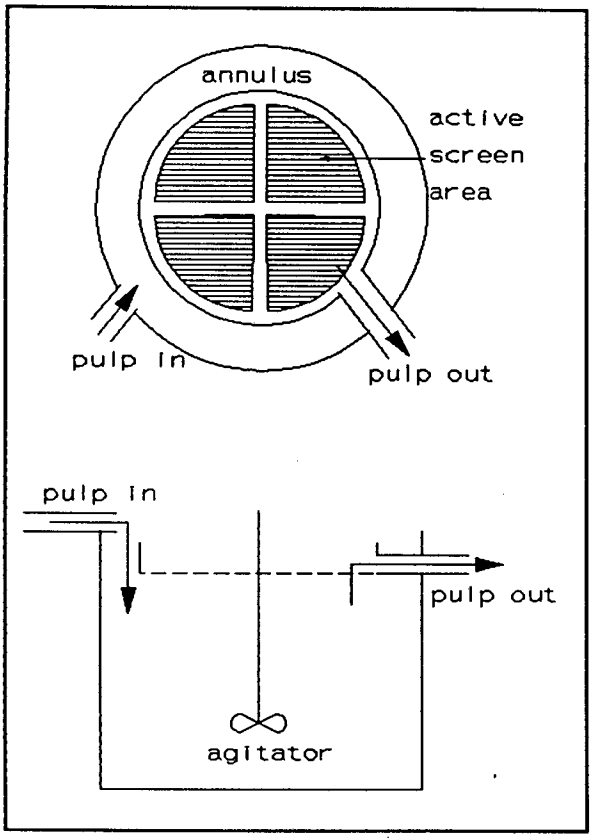


Figure 9 : Top and Front Views of a CIP Contactor

- The carbon screen at the top of the CIP cascade separates the coarse carbon from the pulp in the carbon transfer stream originating in the top-most contactor. The carbon is transferred to the elution section of the plant, while the pulp is returned to the first CIP contactor.

Besides those sections of the plant that were included in the simulation there are a few other processes that are closely related to the simulated processes and influence the functioning of both the CIP and the leach sections through interconnecting streams. Refer to Figure 10 for a representation of the path followed by the gold through the simulated and adjacent sections. Fortunately the interactions between the various parts are quite weak, because of the intermittent nature of the transport of material between them. The sections not simulated include:

- The pre-elution carbon storage: a large tank in which the loaded carbon from the CIP is stored before it can be transferred to the actual elution column.
- The elution column where the carbon is first treated with concentrated acid to remove build ups of inorganic foulants such as calcite. Depending on the type of elution (Zadra or AARL) the carbon will then be eluted using hot, very alkaline, concentrated cyanide solutions after which (in the AARL process used at the plant on which the simulator was based) the carbon will be washed with hot deionized water, to elute the carbon. The eluate (the concentrated gold-cyanide solution), is then taken to the gold retrieval system.

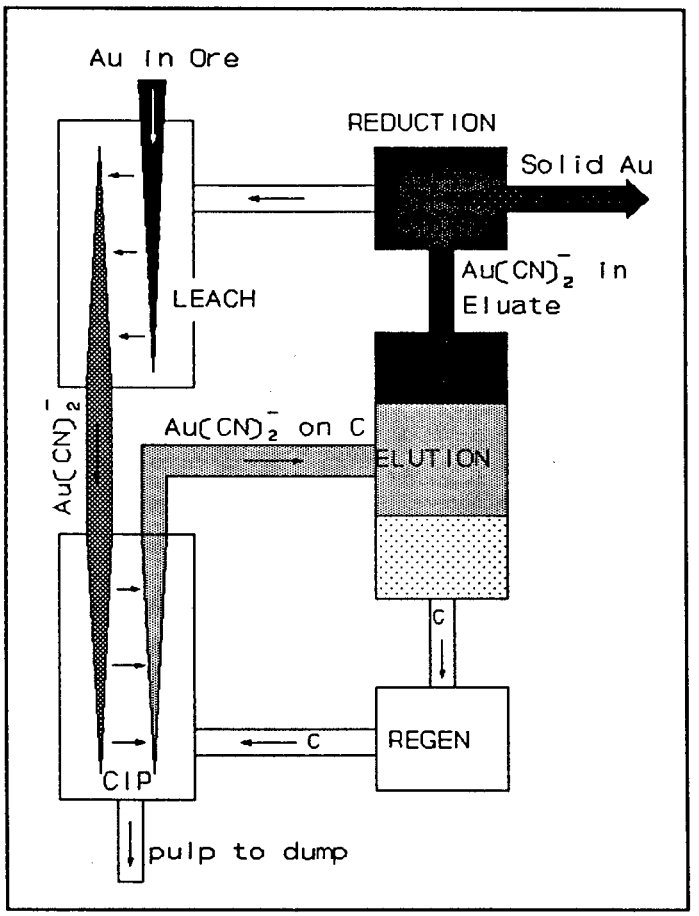


Figure 10 : The Path of Gold Through a Gold Plant

- The gold retrieval system precipitates the gold from the gold cyanide solution. Two processes are commonly used: electroplating employs steel wool cathodes on which the gold will be deposited as the electric current reduces the gold ion in the $Au(CN)_2^-$ complex to metallic gold. The other process, which has been in use for a long time and is used on the present plant, involves sprinkling zinc dust into the

gold cyanide solution. The zinc displaces the gold in the complex, leaving the gold to precipitate out of solution. The resultant solution, which has a low gold content, is called the spent eluate and is pumped back to the top of the leach cascade, so that all the excess hydroxide and cyanide will be put to use.

- The carbon regeneration circuit consists of essentially more storage tanks and a furnace in which the carbon is heated to high temperatures (600 - 700 °C) in a controlled atmosphere. The carbon reacts with the oxygen and new pores are burnt into the carbon interior. The hydro-carbon foulants which collected on the carbon will largely volatilize or decompose under these conditions. The carbon on leaving the furnace will be reactivated. It is quenched in cold water before being mixed with fresh carbon and being pumped back into the bottom-most adsorber.

3.2 SIMULATION APPROACH

The physical process is divided into process units, streams and connections, where the first two categories correspond with their intuitive meanings. A connection constitutes any transfer of information such as signals from a measuring instrument to the controller, or signals from the controller to the final control element. This structure was decided upon as a standard within the Measurement and Control Division to make all flow sheet simulations written in the Division compatible. A process-based approach was used: by definition a stream must originate and terminate at processes. A feed stream therefore has to leave a feed unit, while an exit stream needs to terminate at a sink unit.

The variables used in the simulation were divided into state variables and algebraic variables as suggested by Hulbert (1983). The state variables are all those variables describing the contents of the process units at any time and in terms of which the differential equations describing the changes are written. They are all collected in the state variable vector $\underline{X}$ with their derivatives in vector $\dot{\underline{X}}$. The algebraic variables in contrast include all derived variables (such as volume) and all flows between units (streams and connections). They are needed to calculate the derivatives of the state variables and are all contained in the algebraic variable vector $\underline{A}$.

The sequence of calculation is as follows:

i) Calculate all algebraic variables at time t using the values of the state variables at t, all of which are known. (In flowsheets which are more complicated than this one, eg. with many recycle streams, it may always be possible that some algebraic variable is based on others, which occur later within the algebraic vector. As the integrator was also to be usable in such cases provision was made for the calculation process to be repeated until all algebraic variables have definitely been calculated. A maximum of four such repetitions is allowed before the program exits with an error message.)

ii) Calculate the rates of the chemical reactions using the state variables at time t.

iii) Calculate the derivatives of all state variables at time t, using the algebraic variables and rates of reactions calculated in (i) and (ii). $\dot{\underline{X}} = f(\underline{X},\underline{A}(\underline{X}),t)$.

iv) Calculate the values of all state variables at a later time $t+\delta t$ using a numerical integration method, ensuring that the error in this step does not exceed a specified maximum.

v) Repeat steps (i) to (iv) until the required interval has been covered.

The above approach is called the chunked or simultaneous approach. An alternative approach, called the sequential-modular approach, repeats the above sequence separately for each individual unit over a pre-specified time horizon Δt. This has the advantage that each unit will only take as many integration steps as it needs (eg. a unit with small changes needs only a few large steps, while a unit in which the state variables change rapidly, can proceed with many small steps, without affecting the first unit).

The disadvantage of the sequential-modular approach is that the data from an earlier unit used in the integration of a later unit will not be available at the exact time intervals at which it is needed. This means that an interpolation routine must be included to provide the information as and when it is required. While this is not difficult for a linear process in which later units do not affect earlier ones, it is inefficient in a process such as the CIP cascade, in which there is backward and forward flow between adjacent units. Interaction between such units requires iterative recalculation of later states, so that all the time saved by doing the calculations for individual processes separately is quickly lost.

The sequential-clustered approach (described by Fagley and Carnahan, 1990) uses a hybrid of the two above approaches. It divides the flowsheet into clusters of associated units, which are integrated together, with only the interconnecting streams having to be interpolated. It thereby makes it possible to limit the effect of stiffness in large systems to small clusters.

The integration method used in the simulator is the Bulirsch-Stoer method. It is an explicit method for which the chunked approach was considered the most efficient one in terms of the amount of programming required and the reliability which could be expected.

At present the flowsheet information is entered via a flowsheet data file which has to be written manually. Within the Measurement and Control Division, Mintek, a procedure is to be written which will allow a user to choose the required flowsheet units from a list of available units and to arrange them on the computer screen, complete with connecting streams, as they occur on the plant.

3.3 DYNAMIC MODEL

The equations on which the simulator is based fall into two categories : (i) differential equations which describe how the state variables change with time, and (ii) algebraic equations which describe the dependence of the algebraic variables on the state variables. All state variables, and most algebraic variables, are actually mols of the various species present in the system. Some algebraic variables are derived quantities (such as mol totals, volumes and flows in $mol.s^{-1}$) which are needed to make the results more immediately meaningful. Concentrations (in $mol.m^{-3}$) are not kept explicitly, but are calculated when needed.

In an effort to keep the sizes of the algebraic and state variable vectors as small as possible to save memory space, the species used in the leach and CIP sections are not the same. Rather each section has its own selection of species, with a 'magic box' between the sections which transposes the algebraic variables of the stream leaving the leach onto the CIP feed stream vector (refer to section 3.5.4.5).

3.3.1 Leach Section

The leach section consists of the leach cascade consisting of ten pachucas and the pre-leach tank. The reactions and equations given for the leach below apply equally well to the pre-leach tank, which incorporates exactly the same species and reactions as the leach. The only and significant difference is that no cyanide is present in the pre-leach tank. This prevents all reactions involving cyanide to proceed, leaving only the oxygen dissolution reaction which can proceed. This tank is therefore often described as the pre-aeration tank.

3.3.1.1 Leach Species Table II lists all the species included in the leach section.

Species No.	Chemical Formula	Density ($kg.l^{-1}$)	Mol.Mass ($kg.kmol^{-1}$)
1	H_2O	1,00	18,015
2	SiO_2	2,70	60,085
3	$Ca(OH)_2$	2,43	74,094
4	Ca^{2+}	0*	40,080
5	OH^-	0*	17,007
6	CN^-	0*	26,018
7	O_2 (aq)	0*	31,998
8	Au_f	19,30	196,967
9	Au_s	19,30	196,967
10	$Au(CN)_2^-$	0*	249,003
11	M_f	8,95	63,546
12	M_s	8,95	63,546
13	$M(CN)_4^{3-}$	0*	167,618

Table II : Leach Species with Physical Constants

Note: * all dissolved species are assumed to have negligible volume)

The significance of the subscripts f and s on Au and M is explained below.

3.3.1.2 Leach Mole Balances The differential equations for all species in the leach are written as mole balances. For species j in tank i:

$$\frac{dn_{i,j}}{dt} = \dot{n}_{i-1,j} - \dot{n}_{i,j} + \sum_{m=1}^{M} \alpha_{j,m} r_m(n_{i,1}, n_{i,2}, \ldots, n_{i,N}) \quad \text{for } i=1,\ldots,NT; j=1,\ldots,N \qquad \text{(L-18)}$$

where $\dot{n}_{i,j}$ is the number of mols of j flowing out of tank i,

$\alpha_{j,m}$ is the stoichiometric constant of component j in reaction m, and

r_m is the rate of reaction m which is potentially a function of all n in tank i. (See section 3.3.1.3 for the reaction rate equations.)

$\dot{n}$ is calculated from

$$\dot{n}_{i,j} = v_{i,j} Q_i \frac{\rho_j}{\mu_j} = \frac{n_{i,j}}{V_i} Q_i = \frac{n_{i,j} Q_i}{\sum_{k=1}^{N} \frac{n_{i,k} \mu_k}{\rho_k}}$$

where $v_{i,j}$ is the volume fraction of component j in tank i,

Q_i is the volume flowrate out of tank i,

ρ_j is the density of component j,

μ_j is the molecular mass of component j,

$n_{i,j}$ is the number of mols of species j in tank i, and

V_i is the volume occupied by material in tank i.

3.3.1.3 Leach Reactions Besides the reaction of gold with cyanide, countless other reactions take place in the pulp as its various constituents react with the oxygen, the lime, the water, the cyanide or with each other. As can be seen in Table 1 above, only 13 species have been chosen for the simulation. While this is a limited choice, it is sufficient for a first approximation as all reactions of interest can be described in terms of these species.

The solid phase is assumed to consist of only inert quartz (referred to as SiO_2 in Table II), solid gold and solid 'metal', where 'metal' is a collective term for all the metals which compete with gold for the cyanide and oxygen. It is given a coordination number of 4 to fall within the range of the four main competing metals of the tested ore, viz. silver (in $Ag(CN)_2^-$), copper (in $Cu(CN)_4^{3-}$), nickel (in $Ni(CN)_4^{2-}$) and iron (in $Fe(CN)_6^{2-}$). These

metals are listed in order of their increasing grade in the ore and also in decreasing order of reactivity (ie. even though silver is the rarest of the metals, it is the most likely to react with the cyanide.)

Both gold and metal particles are each assumed to occur in two discrete classes with respect to the rate at which they leach. The first, or fast-leaching, group is directly exposed to the solution and therefore leaches relatively quickly. The other class of particles is assumed to be partially occluded by the gangue material and therefore leaches more slowly. Overall this results in a fast initial rate of leaching followed by a marked decrease as is typically observed. This dual-rate model was suggested by Vetter (1987) as a simplification of the distribution of rate constants as suggested by Loveday et.al.(1973).

The rate equation chosen for the leaching of both gold and metal is based on Habashi's (1966) rate equation, which has the advantage that it is written in terms of the three reactants involved, viz. gold/metal, cyanide and oxygen. According to Habashi (1966) most gold leaches according to Bodländer's first equation:

$$2Au + 4CN^- + O_2 + 2H_2O \rightharpoonup 2Au(CN)_2^- + 2OH^- + H_2O_2 \quad \ldots . \text{(L-2a)}$$

About 10% of the H_2O_2 produced in this reaction is consumed by Bodländer's second reaction (Finkelstein, 1972):

$$2Au + 4CN^- + H_2O_2 \rightharpoonup 2Au(CN)_2^- + 2OH^- \quad \ldots\ldots\ldots . \text{(L-2b)}$$

Overall this results in an equation with rather odd stoichiometric constants:

$$Au + 2CN^- + 0{,}4545O_2 + 0{,}909H_2O \rightharpoonup Au(CN)_2^- + OH^- + 0{,}409H_2O_2$$

$$\ldots\ldots\ldots\ldots . \text{(L-19)}$$

According to Habashi, the rate of gold leaching is:

$$\frac{dn_{Au}}{dt} = \frac{2A_{Au}D_{CN}\text{-}D_{O_2}C_{CN}\text{-}C_{O_2}}{\delta(D_{CN}\text{-}C_{CN^-} + \chi D_{O_2}C_{O_2})} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots . \text{(L-13)}$$

$$= \frac{2A_{Au}}{\delta}\left(\frac{1}{D_{O_2}C_{O_2}} + \frac{\chi}{D_{CN}\text{-}C_{CN^-}}\right)^{-1}$$

$$= \frac{2A_{Au}D_{O_2}}{\delta}\left(\frac{1}{C_{O_2}} + \frac{1{,}5\,\chi}{C_{CN^-}}\right)^{-1} \qquad as \ \frac{D_{O_2}}{D_{CN^-}} \approx 1{,}5$$

The term χ stands for the ratio of cyanide to oxygen (= 2:0,4545 = 4,4) in equation (L-19) above. Dividing by the volume of liquid, V_l, on both sides gives

$$\frac{dC_{Au}}{dt} = \frac{2A_{Au}D_{O_2}}{\delta V_l}\left(\frac{1}{C_{O_2}} + \frac{1{,}5\,\chi}{C_{CN^-}}\right)^{-1}$$

By manipulating the term before the large bracket one can express the rate in terms of the concentration of solid gold in liquid, C_{Au}:

$$\frac{dC_{Au}}{dt} = \frac{6\mu_{Au}D_{O_2}s}{\rho_{Au}\bar{R}_{Au}\delta}C_{Au}\left(\frac{1}{C_{O_2}} + \frac{1{,}5\,\chi}{C_{CN^-}}\right)^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(L-20)}$$

where s is a factor relating the exposed surface of gold A_{Au} to the total surface of the gold particles, and

$\bar{R}_{Au}$ is the average radius of the gold particles.

Similarly one can write the corresponding equation for metal:

$$M + 4CN^- + 0{,}4545O_2 + 0{,}909H_2O \rightharpoonup M(CN)_4^{3-} + OH^- + 0{,}409H_2O_2$$

$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$ (L-21)

which has the rate equation of:

$$\frac{dC_M}{dt} = \frac{6\mu_M D_{O_2}s}{\rho_M \bar{R}_M \delta}C_M\left(\frac{1}{C_{O_2}} + \frac{1{,}5\,\chi}{C_{CN^-}}\right)^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(L-22)}$$

where again χ = 4,4.

A list of all reactions which are included in the leach simulation is given below. The rate constants that are shown, are those used in the simulator. Unless otherwise indicated, they were chosen on the basis of the data from the sampling campaign and other data available from the gold plant. See section 3.3.3 for an explanation on how the constants were chosen.

1) $Ca(OH)_2(s) \rightharpoonup Ca^{2+}(aq) + 2OH^-(aq)$ $\ldots\ldots\ldots\ldots\ldots\ldots$ (L-23)

with the rate equation:

$$r_{Ca(OH)_2} = k_1 C_{Ca(OH)_2} \left(1 - \frac{(C_{Ca^{2+}})(C_{OH^-})^2}{K_{sp}}\right) \quad \text{(L-24)}$$

where $k_1 = 3.10^{-3}.s^{-1}$, and

$K_{sp} = 2{,}937 \cdot 10^{-5}(kmol^1.m^{-3})^3$ is the solubility product of calcium hydroxide.

This reaction indicates how the lime acts as a pH buffer to keep the pH ~10. The concentration of calcium hydroxide is in equilibrium with its two products, Ca^{2+} and OH^-, as determined by the solubility product.

2) $$O_2\,(g) \rightleftharpoons O_2(aq) \quad \text{(L-25)}$$

with rate equation:

$$r_{O_2} = k_2\left(C_{O_2}^{eq} - C_{O_2}\right) \quad \text{(L-26)}$$

where $k_2 = 7{,}621.10^{-5}.s^{-1}$, and

$C_{O2}^{eq} = 0{,}331 \cdot 10^{-6}$ kmol.m^{-3} is the equilibrium concentration of dissolved oxygen in the pulp as measured on the plant.

The form of the equation chosen is a compromise between the behaviour which it was expected to predict and the available information. No data was available on the addition of compressed air, so that the assumption was made that aeration was always more than adequate to make dissolution independent of the amount of air actually present. To prevent the concentration rising above the observed maximum concentration, the equilibrium term had to be included.

3) $$CN^- + \tfrac{1}{2}O_2 \rightleftharpoons CNO^- \quad \text{(L-27)}$$

with a rate equation similar to that proposed by Adams (1990a) but adapted to include the limiting effect of the oxygen concentration:

$$r_{CNO^-} = k_3\, C_{CN^-} \frac{C_{O_2}}{C_{O_2}^{eq}} \quad \text{(L-28)}$$

where $k_3 = 1{,}58.10^{-6}.s^{-1}$, which was interpolated from the selection of constants supplied by Adams for various different cases.

Equations (L-19) to (L-22) are then written twice, once for the fast leaching fraction and once for the slow leaching fraction:

4 and 5)

$$Au_{fls} + 2CN^- + 0{,}4545O_2 + 0{,}909H_2O \rightleftharpoons Au(CN)_2^- + OH^- + 0{,}409H_2O_2$$

. . . . . (L-19a/b)

with rate equations:

$$r_{Au_{fls}} = k_{4/5}\, C_{Au,fls} \left(\frac{1}{C_{O_2}} + \frac{6{,}6}{C_{CN^-}} \right)^{-1} \quad \text{. . . . . (L-20a/b)}$$

where $k_4 = 1{,}215.10^3.m^3.kmol^{-1}.s^{-1}$, and

$k_5 = 8{,}501.10^1.m^3.kmol^{-1}.s^{-1}$

6 and 7)

$$M_{fls} + 4CN^- + 0{,}4545O_2 + 0{,}909H_2O \leftharpoondown M(CN)_4^{3-} + OH^- + 0{,}409H_2O_2$$

. . . . . (L-21a/b)

with rate equations:

$$r_{M_{fls}} = k_{6/7}\, C_{M,fls} \left(\frac{1}{C_{O_2}} + \frac{6{,}6}{C_{CN^-}} \right)^{-1} \quad \text{. . . . . (L-22a/b)}$$

where $k_6 = 2{,}036.10^3.m^3.kmol^{-1}.s^{-1}$, and

$k_7 = 1{,}169.10^3.m^3.kmol^{-1}.s^{-1}$

The side reactions which consume oxygen and cyanide are represented by (L-21a and b) and by (L-27). This limited selection is again sufficient for a first approximation.

A reaction which was earlier considered for inclusion in the simulator, is the dissociation of NaCN to CN^- and Na^+. This reaction is fast in comparison to the leaching reactions and the hydrodynamics of the leach. It was thus assumed to have already gone to completion in the cyanide feed unit before the cyanide stream is mixed with the pulp.

3.3.1.4 Leach Hydrodynamics The leach cascade is arranged in such a way that the pulp which is fed into the first leach tank flows down the cascade under gravity. The tanks themselves are arranged at the same height, though, and all interconnections between the tanks are also on a common level about 3 m below the top of the pachucas. This means that the pulp levels in all the ten leach tanks are dynamically dependant on each other. This arrangement gives the leach circuit a potentially very large buffering capacity. Regardless of whether this is consciously used to control the feed flow to the CIP or not, any fluctuations in the feed to the leach will have been reduced significantly before reaching the CIP.

The interaction of the levels was regarded important enough to be included in the model. Levels in the leach pachucas were therefore not taken as being constant, but are calculated from the volumes of the individual species in the tank. The flow from one tank to the next is represented as an interaction between the two volumes:

$$Q_i = B(V_i - V_{i+1}) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(L-29)}$$

where B is the buffering constant.

In the case where the next tank in line has not filled sufficiently for interaction to occur, the above equation reduces to

$$Q_i = B(V_i - V_{max}) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(L-30)}$$

where V_{max} is the volume of the tank up to the top of the weir. This is also the equation which is used for the last tank, which obviously has no succeeding tank with which to interact.

3.3.2 CIP Section

3.3.2.1 CIP Species

Species No.	Chemical Formula	Density ($kg.l^{-1}$)	Mol.Mass ($kg.kmol^{-1}$)
1	H_2O	1,00	18,015
2	SiO_2	2,70	60,085
3	CN^-	0*	26,018
4	O_2 (aq)	0*	31,998
5	$Au(CN)_2^-$	0*	249,003
6	$M(CN)_4^{3-}$	0*	167,618
7	C-granules	1,40	12,011
8	C-fines	1,40	12,011
9	$q_{Au(CN)2,fin}$	0**	249,003
10	$q_{Au(CN)2,m}$	0**	249,003
11	$q_{Au(CN)2,b}$	0**	249,003
12	$q_{M(CN)4,fin}$	0**	167,618
13	$q_{M(CN)4,m}$	0**	167,618
14	$q_{M(CN)4,b}$	0**	167,618
15	$q_{CN,fin}$	0**	26,018
16	$q_{CN,m}$	0**	26,018
17	$q_{CN,b}$	0**	26,018
18	C-transfd	0+	12,011

Table III : CIP Species with Physical Constants

Notes: * all dissolved species are assumed to have negligible volume.

** all adsorbed species are assumed to have negligible volume.

+ this variable is only needed to keep track of how much carbon has been transferred to each particular tank. It should in essence be an algebraic variable, but is easier to handle as a state variable.

3.3.2.2 CIP Mol-Balances As in the leach, all differential equations in the adsorption section are mol-balances. They are essentially the same as those in the leach except for the extra terms for the transfer streams.

For species j in tank i:

$$\frac{dn_{i,j}}{dt} = \dot{n}_{p,i-1,j} - \dot{n}_{p,i,j} + \dot{n}_{t,i+1,j} - \dot{n}_{t,i,j} + \sum_{m=1}^{M} \alpha_{j,m} r_m(n_{i,1}, n_{i,2}, \ldots, n_{i,N}) \quad \text{for } i=1,\ldots NT; j=1,\ldots N \quad \text{. (C-14)}$$

where $\dot{n}_{p,i,j}$ is the number of mols of j flowing out of tank i in the pulp stream,

$\dot{n}_{t,i,j}$ is the number of mols of j flowing out of tank i in the carbon transfer stream,

$\alpha_{j,m}$ is the stoichiometric constant of component j in reaction m, and

r_m is the rate of reaction m which is potentially a function of all n in tank i.

$\dot{n}_{p,i,j}$ and $\dot{n}_{t,i,j}$ are both calculated using

$$\dot{n}_{\xi,i,j} = v_{i,j} Q_{\xi,i} \frac{\rho_j}{\mu_j} = \frac{n_{i,j}}{V_i} Q_{\xi,i} = \frac{n_{i,j} Q_{\xi,i}}{\sum_{k=1}^{N} \frac{n_{i,k} \mu_k}{\rho_k}} \qquad \xi \in \{t,p\}$$

where $v_{i,j}$ is the volume fraction of component j in tank i,

$Q_{p,i}$ is the volume flowrate out of tank i in the pulp stream,

$Q_{t,i}$ is the volume flowrate out of tank i in the carbon transfer stream,

ρ_j is the density of component j,

μ_j is the molecular mass of component j,

$n_{i,j}$ is the number of mols of species j in tank i, and

V_i is the volume occupied by material in tank i.

These equations are very flexible and allow the movement of pulp and carbon to be simulated within the cascade. As long as the ṅ-terms are set to zero when the pulp or transfer streams are cut, this equation will automatically take care of the various transfer schemes, overflows etc. as is discussed below in the section on hydrodynamics.

3.3.2.3 CIP Reactions Again a great variety of reactions occur simultaneously in the adsorption section of a gold plant. Only a few representative ones have been chosen in this simulation to present an approximate picture of what happens. The choice of unreferenced kinetic constants is again described in section 3.3.3.

The process of adsorption may be described by the following stoichiometric equation:

$$Au(CN)_2^- \ (aq) \rightleftharpoons Au(CN)_2^- \ (\downarrow) \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(C-15)}$$

where $\downarrow$ refers to the adsorbed species.

The rate of adsorption is calculated using a slightly modified version of Nicol's linear isotherm adsorption rate equation (C-4):

$$r_{Au(CN)_2^-} = k\left(C_{Au(CN)_2^-} - Kq_{Au(CN)_2^-}\right)n_C \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(C-16)}$$

The modification is necessary as the concentration of carbon in the pulp varies and can be quite low during carbon transfers. According to Nicol's original rate equation the amount of gold adsorbed from solution would not be affected by a lack of carbon but that can obviously not be the case.

In experiments it was observed that fast adsorption occurs initially on the surface and in the macropores of the carbon. The rate of adsorption then slows down significantly when the only remaining sites are located in the micropores. To take this observed effect into account, Vetter's (1987) approach was used in which it is assumed that part of the carbon contains only macropores, which are filled quickly. The rest of the carbon contains only micropores for which loading is slow. As the aurocyanide in each pore not only adsorbs independently, but can also desorb independently, the number of mols stored in each kind of pore needs to be stored separately. A stoichiometric equation can then be written for each adsorbed species :

$$Au(CN)_2^- \ (aq) \rightleftharpoons Au(CN)_2^- \ (\downarrow_j) \qquad j \in \{m,b\} \quad \ldots\ldots\ldots \text{(C-15a/b)}$$

where $\downarrow_m$ refers to adsorption in the macropores,and

$\downarrow_b$ refers to adsorption in the micropores.

The loading of a species on carbon is calculated by dividing the number of loaded mols of the species by the number of mols of carbon (or the volume of carbon, etc.). Loadings are therefore automatically assumed to be average loadings and no loading distribution is considered within a tank. As Willacott et.al.(1990) noted, this approximation is acceptable as long as the loading rate equation is linear in the loading term.

Attrition of the carbon is a major source of gold loss on a running plant (Sorensen, 1989). The breakage of carbon particles was thus included in the simulation and is described as follows:

$$n_{C\text{-}granules} \rightarrow n_{C\text{-}fines} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \textbf{(C-16)}$$

with the rate equation as suggested by Whyte et.al.(1990):

$$r_C = k_8 C_{C\text{-}granules} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \textbf{(C-17)}$$

where $k_8 = 1{,}30.10^{-4}.s^{-1}$

The adsorption of $Au(CN)_2^-$ on the fine carbon fraction was also monitored. The equilibrium loading capacity of fine carbon is the same as that of the coarse carbon, but adsorption onto and desorption from fine carbon is much faster because of the smaller diameter of the fine carbon particles. The fine carbon is therefore treated as a single medium of high rate micropores. In total there are then three loading terms for every species as shown in Table 3 above and each has the rate equation:

$$r_{Au(CN)_2^-,j} = k_{9,j}\left(C_{Au(CN)_2^-} - K_{9,j} q_{Au(CN)_2^-,j}\right) n_{C,j} \qquad j \in \{m,b,fin\} \quad \textbf{(C-18a/b/c)}$$

where $k_{9,m} = 4{,}393.10^{-4}$ m^3.kmol^{-1}.s^{-1}, $K_{9,m} = 0{,}1.6{,}513.10^{-6}$ kmol.m^{-3}

$k_{9,b} = 2{,}196.10^{-4}$ m^3.kmol^{-1}.s^{-1}, $K_{9,b} = 0{,}9.6{,}513.10^{-6}$ kmol.m^{-3}

$k_{9,fin} = 4{,}393.10^{-4}$ m^3.kmol^{-1}.s^{-1}, $K_{9,fin} = 1{,}0.6{,}513.10^{-6}$ kmol.m^{-3}

The cyanide complex of the competing metal species also loads onto carbon.Its rate of loading is slower than that of gold and its equilibrium capacity on the carbon is much lower:

$$r_{M(CN)_4^{3-},j} = k_{10,j}\left(C_{M(CN)_4^{3-}} - K_{10,j} q_{M(CN)_4^{3-},j}\right) n_{C,j} \qquad j \in \{m,b,fin\} \quad \textbf{(C-19a/b/c)}$$

where $k_{10,m} = 9{,}0.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{10,m} = 0{,}1.1{,}2.10^{-3}$ kmol.m^{-3}

$k_{10,b} = 4{,}5.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{10,b} = 0{,}9.1{,}2.10^{-3}$ kmol.m^{-3}

$k_{10,fin} = 9{,}0.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{10,fin} = 1{,}0.1{,}2.10^{-3}$ kmol.m^{-3}

Similarly, the free cyanide ion loads onto the carbon as well, but the carbon is again more selective towards gold:

$$r_{CN^-,j} = k_{11,j}\left(C_{CN^-} - K_{11,j} q_{CN^-,j}\right) n_{C,j} \qquad j \in \{m,b,fin\} \quad \ldots\ldots \textbf{(C-20a/b/c)}$$

where $k_{11,m} = 2{,}0.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{11,m} = 0{,}1.1{,}5.10^{-3}$ kmol.m^{-3}

$k_{11,b} = 1{,}0.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{11,b} = 0{,}9.1{,}5.10^{-3}$ kmol.m^{-3}

$k_{11,fin} = 2{,}0.10^{-5}$ m^3.kmol^{-1}.s^{-1}, $K_{11,fin} = 1{,}0.1{,}5.10^{-3}$ kmol.m^{-3}

All the different reactions of cyanide (Adams, 1990a) are accounted for by the following one reaction which was also used for the leach simulation.

$$CN^- + \frac{1}{2}O_2 \rightarrow CNO^- \quad \text{.....(C-21)}$$

Because this reaction is catalyzed by carbon, though, it proceeds at a faster rate than the same reaction in the leach, where no carbon is present. The rate equation is an equation suggested by Adams (1990a) modified to account for the need of oxygen in the production of cyanate. As the presence of oxygen is included only as a fraction of concentration over equilibrium concentration, it was still possible to use a rate constant interpolated from the rate constants supplied in the paper by Adams:

$$r_{CNO^-} = k_{12}\, C_{CN^-} \frac{C_{O_2}}{C_{O_2}^{eq}} \quad \text{.....(C-22)}$$

where $k_{12} = 1{,}3.10^{-5}.s^{-1}$

3.3.2.4 CIP Hydrodynamics The adsorption contactors are much smaller than the leach pachucas. They are arranged at successively lower heights above ground level so that the pulp flows down the cascade by gravity. The levels in the various tanks are independent of each other and each is only affected by the amount of pulp flowing into the tank.

At periodic intervals carbon has to be transferred up the cascade. For this purpose carbon transfer pumps are switched on which move pulp together with the associated carbon to next contactor above. The pulp drains back through the carbon screen, but the carbon is held back by the screen and has thus been transferred to a tank with higher solution concentrations of gold-cyanide.

The carbon screens make the hydrodynamics more complicated. Not only do they present a resistance to the flow of the pulp out of the tank, but they also tend to block and overflow, thereby allowing the loaded carbon to pass downstream.

Under normal circumstances, the amount of pulp above the screen is negligible, and it is therefore assumed that as soon as the pulp has passed through the screen it is already in

the pulp stream to the next tank.

The diagram in Figure 11 shows the horizontal carbon screen during normal operation. The difference in heights (Δh) ensures enough hydrostatic pressure to force the pulp through the screen, while the carbon particles are too large to pass through the screen.

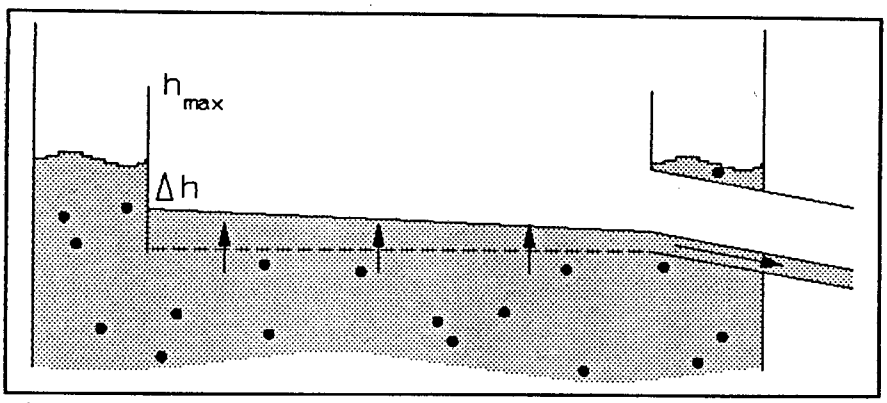


Figure 11 : The Horizontal Carbon Screen

But when a tank gets too full, the following happens:

1) The hydrostatic pressure becomes too great and the carbon, instead of being mixed into the pulp is pressed against the screen. Individual holes are covered by carbon pieces until the entire screen becomes blocked.

2) The pulp level in the annulus around the screen rises, without any pulp flowing to the next tank.

3) Once the level rises above h_{max} the pulp overflows into the area above the screen and from there to the next tank taking carbon with it.

4) The operator then has to close the exit valve to the next tank to allow the level above the screen to rise.

5) When the levels in the annulus and above the screen equalize (roughly h_{max}), the feed valve to the tank must also be closed. The pressures above and below the screen are then also equalized and the screen unblocks.

6) The exit valve is opened to allow the screen and the tank to empty.

7) Once the level has dropped far enough, the feed valve is opened to allow normal operation again.

A potential problem with leaving the feed valve to any tank closed for too long, is that

the screen in the tank before may overflow, requiring its own feed valve to be closed. This happens because the volumes of both the screen and of the annulus around the screen are relatively small. A single blocked screen may therefore cause the successive closure of all tanks above it in the cascade, which will affect the production negatively. The option of opening the feed valve to a blocked tank earlier to prevent overflow of the previous tank simply causes the screen to reblock, and is therefore also not a solution to the problem.

The amount of carbon carried downstream during such an overflow could potentially take quite a large amount of retrieved gold with it, especially if the overflow occurred in one of the earlier stages. The carbon not only carries the gold downstream with it, but if the solution concentration in the next tank is sufficiently much lower, gold may start desorbing from the carbon, increasing the solution losses of gold as well.

The screens are most likely to block during carbon transfers, as the volume of pulp which normally passes through the screen is augmented by the extra pulp which is carried into the tank by the carbon transfer stream. More pulp than usual has to drain via the screen into the next tank, which causes the level in the tank to rise. The extra pressure on the screen increases the probability of a blockage occurring. When the screen does get blocked, it is common practice to stop the transfers both into and out of the affected contactor.

Various transfer schemes have been used in practice or in simulators. These include:

- **Simultaneous transfers** along the whole cascade. The advantage of this scheme is that, provided the transfer flowrates are the same, it should be easy to ensure that the carbon profile along the cascade remains constant. It also disturbs the cascade for only a short time.
- **Sequential transfers starting at the top.** The advantage of this scheme is that the carbon in each tank is not mixed with less loaded carbon before it is pumped to the next tank. This prevents short-circuiting of carbon, ie carbon particles moving more than one tank during a single transfer cycle. The disadvantage is that the cascade is disturbed for a long time, during which at least one tank contains less than

its normal amount of carbon.

- **Sequential transfers starting from the bottom.** While the short-circuiting problem is aggravated by this transfer scheme, the time needed for transfers is reduced because of the higher carbon concentration in the tank from which carbon is being transferred.
- **Continuous transfers.** In this scheme pumps are kept going continuously, but at a reduced flowrate. While this permanently disturbs the process, it is the only transfer mechanism that could potentially allow the CIP section to reach a steady state. All other schemes can at best only reach a pseudo or cyclic steady state, in which the loading curve of one cycle will be exactly the same as the next.
- **Instantaneous transfers.** All carbon is transferred from one tank to the next at the same instant, or during a negligibly short time. This was the preferred method of transfer in pilot plants and because of its ease in simulation, was the preferred method of early simulators. Recently the carousel configuration of adsorption vessels (Whyte et.al,1990) has allowed complete nearly-instantaneous transfers: the point of fresh feed addition can be moved from tank to tank, so that the carbon does not need to be moved at all. The advantage of this transfer method is that the cascade is disturbed for a minimal period of time. If the transfers are complete, as described above, then short-circuiting and distributions of loadings are prevented.
- **Random transfers** are most likely to occur in practise. These are likely to be most inefficient, as they prevent even a cyclic steady state from being achieved.

The transfer schemes which have been incorporated into the present simulation are the simultaneous, the continuous, the consecutive from the top and plant recorded (near random) transfer methods. The efficiencies of the various schemes are discussed later.

3.3.3 Rate Constants

A sampling campaign was carried out on the plant used as a basis for the simulator in September 1991. Samples were taken from the feed to the leach, various positions along the leach and adsorption cascades and from the stream flowing to dump. These samples

were filtered to stop all reactions and analyzed at Mintek for gold, cyanide and metals contents. Dissolved oxygen levels and pH were also monitored both before and during the sampling campaign.

The results collected on the plant were not in the correct form for a deep mathematical analysis or curve fitting. It was used instead to guide the choice of approximate kinetic constants for the various reactions. The importance here lay more in getting the relative shapes of the curves right, rather than ensuring that the numbers fitted exactly.

In the leaching reaction, for instance, it is important to take the relative amounts of the gold and metal into account which will leach, as well as the relative rates of the gold and metal leaching process. As was explained before, the 'metal' species, M, is an imaginary metal, which sums up the effect of all the competing metals, the most important of which are silver, copper, nickel and iron. These metals behave quite differently and the approach of lumping them all into one makes it easy to sum up their effect on cyanide and oxygen consumption. From the normalised plant data it was evident (Figure 12), that even though the competing 'metal' occurs at a far higher concentration in the ore than gold, the gold dissolves much faster and to a much greater extent.

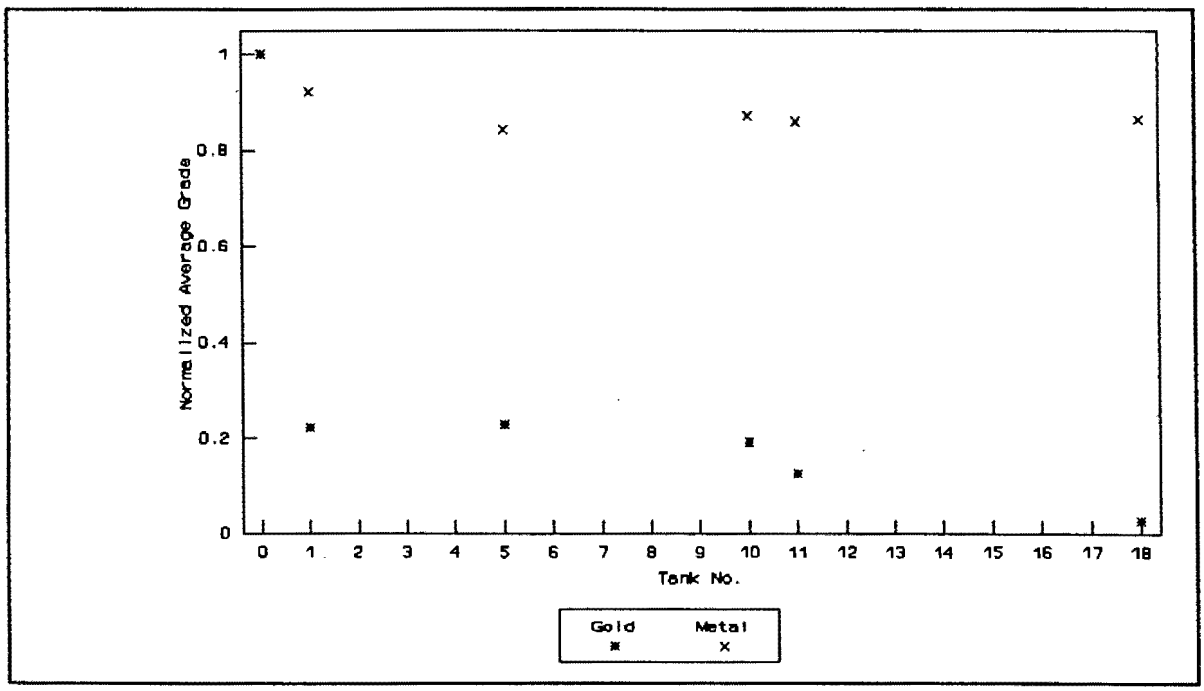


Figure 12 : Normalized Gold and Metal Profiles in the Leach (Plant Data)

In the above diagram tank 0 is equivalent to the feed grade, tanks 1 to 10 are the leach pachucas, while tanks 11 to 18 are the CIP contactors.

The different rates of leaching are taken into account by the choice of constants in the model (see Figure 13 which shows the normalised leaching profiles of gold and metal along the cascade). Two simplifying assumptions have had an effect on the shape of the profile: firstly only the dissolvable fractions of gold and metal are included, and secondly all leaching is assumed to occur only while the pulp is actually resident in the leach cascade. The feed grade of gold is therefore slightly higher in reality while the true feed grade of the competing metal is much higher than indicated in the model. Applying these conditions yields a metal-cyanide concentration roughly ten times as large as that of gold-cyanide concentration, as was recorded on the plant.

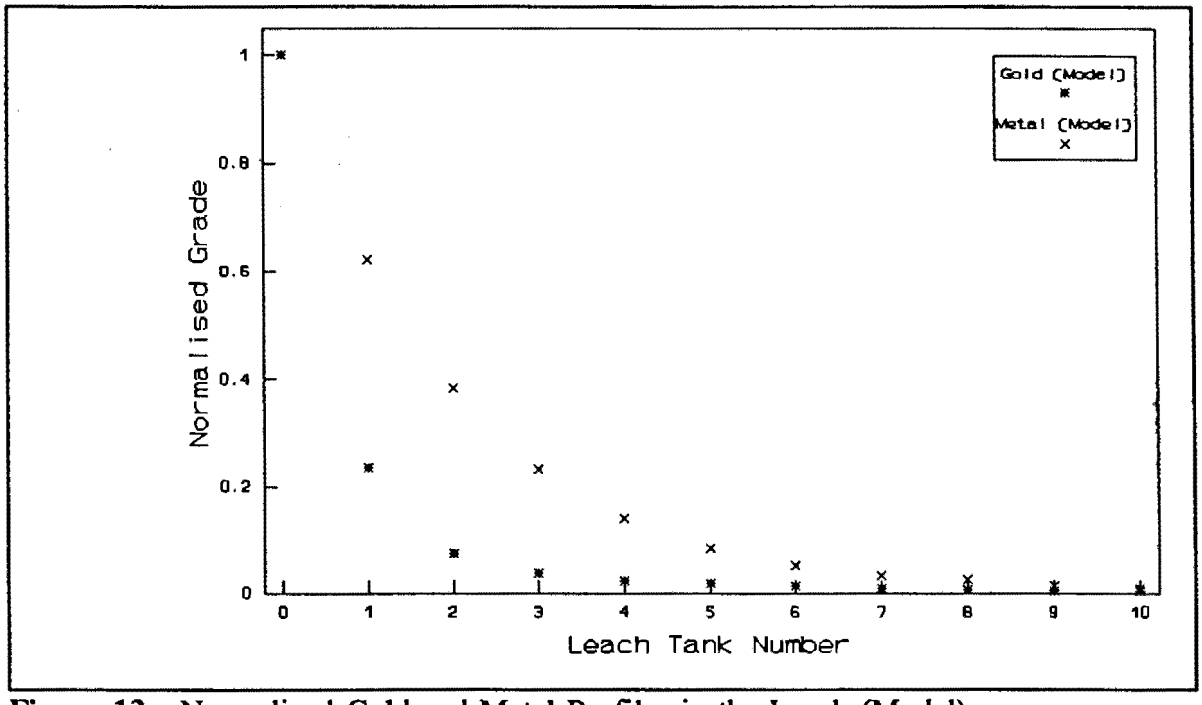


Figure 13 : Normalized Gold and Metal Profiles in the Leach (Model)

Besides the consumption of cyanide by the formation of the gold and metal complexes, some cyanide is also lost in its reaction with oxygen to give cyanate, in its hydrolysis to HCN and various other reactions as discussed by Adams (1990). As he suggests that the cyanate-producing reaction is the most important of the side reactions, it was assumed for simplicity that this was the only other reaction involving cyanide. A rate constant was

therefore chosen so that the concentration of free cyanide corresponded approximately to an average value recorded during the sampling campaign.

The rate constant of oxygen dissolution reaction was chosen such that the simulated profile of dissolved oxygen concentration in the cascade corresponded to the one recorded on the plant.

For the adsorption section the choice of constants was also guided by the results from the sampling campaign. In the adsorption reaction it was found, that the loading capacity of gold cyanide on the activated carbon was much higher than for all the other metals combined, and the rate of $Au(CN)_2^-$ adsorption was much higher than for $M(CN)_4^{3-}$. The desorption constant, K, which governs the loading equilibrium was therefore chosen to be much smaller for gold cyanide than for the metal cyanide species. In contrast the rate constant for gold adsorption mirrors the faster loading of gold by being about five times as large as the rate constant for the metal loading.

The kinetic and loading terms for each species on the three available types of sites (micropores on the fines and micro- and macropores on the coarse carbon) were linked to make their determination easier. For instance, the rate constant for the adsorption on fast-filling sites (micropores on the fine carbon and macropores on the coarse carbon) are assumed equal and double the rate constant for the slow filling sites (the micropores on the coarse carbon). Similarly the equilibrium loading capacity of a carbon must be the same for a single species, regardless of whether the carbon is fine or coarse. A single loading constant (eg. 6,513 kmol of carbon per m^3 of solution for gold in equation C-16) is chosen for each species and is scaled according to the relative percentage of pores in the carbon fraction : All pores in the fines are assumed to be micropores, so for the fines fraction the loading constant is multiplied by 1. In contrast, the coarse carbon contains 90% micropores and 10% macropores. Therefore of the total loading capacity for each species on coarse carbon, 90% is reserved for sites in the micropores, hence $K_b = 0{,}9.K_{tot}$.

Furthermore, it seems from analyses of adsorption behaviour that the equilibrium

capacities of individual species is dependent on the loading of all species present. The cyanide loading was therefore included for possible later incorporation into a competitive loading model. For this work analyses of CN^- on carbon were not available and therefore no information on either its equilibrium loading or rate of loading was available. The constants for cyanide were thus guessed and have no physical significance.

3.4 NUMERICAL INTEGRATION

The integration of the differential equations within the simulator is performed by a variable step-length Bulirsch-Stoer method. It is a highly efficient explicit method for smooth systems and was adapted for the present simulator to be able to deal with discontinuities.

3.4.1 The Bulirsch-Stoer Integrator

This relatively new integration method is the suggested method for non-stiff systems of ordinary differential equations (ODEs) in Press et.al.'s (1986) book "*Numerical Recipes*". Most information in this section and the original versions of some of the integrator subroutines were taken from that book.

The Bulirsch-Stoer method uses a modified-midpoint method to generate a number of estimates of the state variable vector at the end of a pre-specified time step using an ever increasing number of sub-steps. A Richardson extrapolation is then performed on these estimates to use the information available from previous estimates to extrapolate to the result at an infinite number of substeps. This allows the method to safely take relatively large steps using far fewer function calls than a fourth-order Runge-Kutta method would use.

An explicit integration method was thought to be more practical for integrating a system with such a large number of variables as the present one. An implicit method, such as predictor-corrector, needs data from a few previous steps for its calculation, which have to be kept in memory. This could pose a difficulty in a system with many variables, where

a large percentage of the available memory space will be used up by the stored values of previous integration results.

The modified mid-point formulae are:

$$\begin{aligned} z_0 &\equiv x(t) \\ z_1 &= z_0 + h\dot{x}(t,z_0) \\ z_{m+1} &= z_{m-1} + 2h\dot{x}(t+mh,z_m) \qquad m \in \{1,2,\ldots,n-1\} \\ x(t+H) &\approx x_n \equiv \frac{1}{2}[z_n + z_{n-1} + \dot{x}(t+H,z_n)] \end{aligned} \tag{C-1}$$

where z_0 is the value of x at the beginning of the integration interval, at t=t,

z_m is the intermediate function estimate at the end of sub-step m,

h is the distance between successive z's,

H is the total length of the integration step (=n.z), and

x_n is the final estimate of the value of x at the end of the integration interval.

If estimates of the complete state variable vectors $\underline{x}_n$ have been calculated for a number of different sub-step sizes, they are compared and by using a Richardson extrapolation a new vector $\underline{x}_{n\infty}$ is calculated, which is anticipated to be the vector of values which would have been determined if an infinite number of substeps had been used. (The next section explains how this extrapolation works.)

The error in calculation is estimated by dividing each component of the local truncation vector $\underline{x}_{err}$ by a corresponding value in a scale vector (usually a function of an earlier version of $\underline{x}(t)$ plus its derivative multiplied by the length of the integration interval - see the section on errors) and then finding its largest component. If the error is too large (this is user definable) then the integration will be repeated with the interval divided into six subintervals, etc. An ever increasing number of subintervals n_i is used, where the suggested sequence was $n_i \in \{2,4,6,8,12,16,24,32,48,64,96\}$. As each function call in the present simulator involves a large number of calculations, this was reduced to $n_i \in \{2,4,6,8, 10,12\}$ to speed up the integration.

If at any stage the error is small enough, $\underline{x}_{n\infty}$ is accepted as correct and the simulation

proceeds to the next interval. If after the maximum number of subdivisions the error is still too large, the size of the interval is reduced significantly, and the integration will be reattempted. If the error is very large at any stage, the program assumes that a discontinuity has been encountered. The time interval and the relevant information at the start of the interval are passed to a subroutine which locates and crosses the discontinuity (see the section on discontinuities: 3.4.4).

3.4.2 Extrapolation

Once the end of an integration interval is reached, and an $\underline{x}_n$ has been calculated for a new number of subintervals, n_i, (so that $\underline{x}_n = \underline{x}_n(i)$) it is passed to the extrapolation routine, to allow calculation of an estimate of $\underline{x}_{n\infty}$. $\underline{x}_{n\infty}$ is the vector of state variables which is attainable if the integration interval is divided into an infinite number of sub-intervals.

The extrapolation is done by filling in the following table for each component of the vector $\underline{x}_{ni}(i)$, with the number of terms in line i equal to the number of extrapolation attempts i+1 :

$$
\begin{array}{lll}
n_0 = 2: & a_0^0 & \\
n_1 = 4: & a_1^0 & a_0^1 \\
n_2 = 6: & a_2^0 & a_1^1 \quad a_0^2 \\
\vdots & \vdots & \vdots \\
n_5 = 12: & a_5^0 & a_4^1 \quad a_3^2 \ldots a_0^5
\end{array}
$$

The first term after the colon is simply the new value of x(i), ie $a_s^0 = x(s)$. Each other term is calculated from those above and to the left of it by the following formula (Lambert, 1976):

$$a_s^r = a_{s+1}^{r-1} + \frac{a_{s+1}^{r-1} - a_s^{r-1}}{\left(\frac{n_{r+s}}{n_s}\right)^2 \left(1 - \frac{a_{s+1}^{r-1} - a_s^{r-1}}{a_{s+1}^{r-1} - a_{s+1}^{r-2}}\right) - 1} \quad \text{. . . . . (S-2)}$$

$r = 1,2,...5$
$s = 0,1,...5$

where $a_s^{-1} = 0$.

The extrapolated value $x_{n=}(i)$ is the number on the right end of row i, a_0^i.

The local truncation error associated with the extrapolated value a_0^i is the second term in (S-2) so that $E = a_0^i - a_1^{i-1}$ (ie. the difference between the last term in row i and the term to the left of it).

3.4.3 Step-Size Selection

The method for choosing the step-size of the next step used in the simulator and described here is taken largely from Press et.al.(1986) but was adapted slightly using ideas by Gear and Østerby (1984).

The size of the next integration step is found by scaling the size of the present step according to the amount of effort involved in integrating across it. This amount of effort is calculated by comparing the number of integration attempts i (using the associated number of sub-steps n_i) which were needed to reduce the error to an acceptable level, with a desired or standard number of attempts i_s:

- if $i = i_s$ then the next step will be decreased slightly,
- if $i = i_s - 1$ then the next step will be increased slightly,
- otherwise, if the number of the successful attempt lies further from the standard number, the step size will be increased or decreased by a scaled amount. This amount depends on the ratio of the number of substeps which should have been used to the number which were actually used.

In the case where the integration over the previous interval failed (ie if the error was still too large even when the maximum number of substeps was used), the step-size needs to

be decreased substantially. (If a discontinuity had been discovered, a different approach would be used.)

As a safety precaution a minimum step size is stipulated. This prevents the simulator from crashing on rough spots, where it would try to cut the step-size down further and further until it became zero.

3.4.4 Discontinuities

When the error within an integration interval is very large (see next section on errors) so that a discontinuity is suspected to lie in the interval, the method suggested by Gear and Østerby (1984) is used to find and cross it.

An interval-halving technique is used to narrow down the range in which the discontinuity lies. The process of halving the interval continues until the algorithm decides that the error involved in crossing the discontinuity will be of acceptable size. The magnitude of this final step depends on the order of the discontinuity. For instance a first order discontinuity is one with a finite jump in the function value as shown in Figure 14. This is the most difficult type of discontinuity to cross and if the order of a discontinuity cannot be determined, it is assumed to be first order.

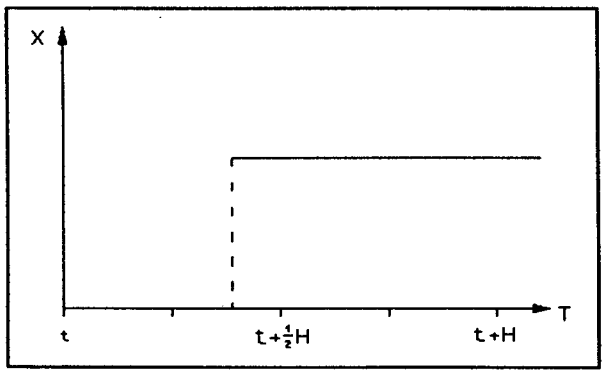


Figure 14 : A First Order Discontinuity

(It must just be mentioned here that this method works only for a change in the state variable x from zero. This means that if the value of the state variable was not zero, a function would have to be fitted to the previously known values of the state variable and

this fitted function would then have to be subtracted out. Luckily in the present model, all discontinuities actually do involve changes from zero and the fitting of functions was not necessary.)

All discontinuities of order larger than one involve only a change in gradient without the finite jump. The second order discontinuities involve a sudden change of gradient (solid line in Figure 15), while any higher order discontinuity involves a gradual change, as shown below (dashed line). Discontinuities of order larger than two do not present a problem for the integrator and can often be crossed by simply cutting down the step size.

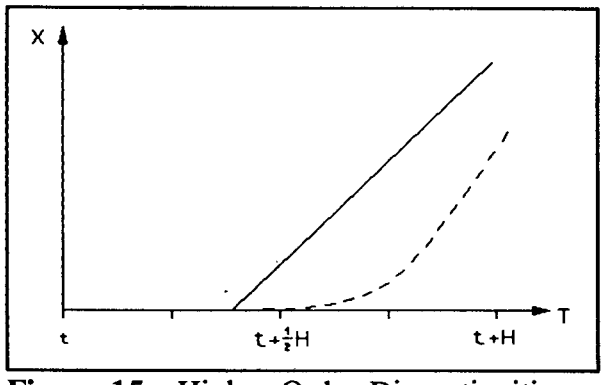


Figure 15 : Higher Order Discontinuities

The sequence of successes and failures is used to decide on the most likely order and position of the discontinuity. (For the detailed decision process used in this method, refer to the article of Gear and Østerby (1984).) A failure occurs when the integration over an interval (eg. length H) and the integration over the two half-intervals give different results, which indicates that the discontinuity lies within the interval H. A success is the opposite case where the two integration attempts yield very similar answers, indicating that no discontinuity lies within the interval.

The need to decide on the order of the discontinuity arises out of the possible saving of computational effort and time when discontinuities are of order greater than one. As mentioned above, first order discontinuities are the most difficult to cross : the error incurred when crossing a first order discontinuity is far greater than for higher order discontinuities and therefore the step in which the discontinuity can be crossed must be much shorter. This means that far more effort needs to be spent on locating the position

of the discontinuity.

Second order discontinuities are easier to cross as the error involved is relatively small and the integration step across the discontinuity can be relatively large. A further advantage of a second order discontinuity is that under certain special circumstances its exact position may be estimated reliably. Once its position has been determined, the integrator can step right up to the discontinuity and cross it, which may potentially save a great deal of computational effort.

Third and higher order discontinuities pose no problem to the integrator. The error involved in crossing such a discontinuity is very small and the crossing can be done in large steps. Similar processes for locating the exact position of the discontinuities exist but the increased complexity in the mathematics is usually not worth the trouble considering the ease with which these discontinuities are crossed.

For each order of discontinuity a method exists of predicting the size of the step with which the discontinuity can be crossed without exceeding the permitted error magnitude. Apart from knowing what order the discontinuity has it is also necessary to calculate the divided differences (DD's) associated with previously attempted integration steps. The first DD is a simple gradient calculated across a single interval. The second DD is the change in gradient calculated over two consecutive intervals.

Once a discontinuity, regardless of its order, has been crossed, the integration has to be restarted. As an explicit integration method is used in this simulator, restarting is not a problem, and normal integration can resume immediately after the discontinuity has been crossed.

3.4.5 Errors

At every integration attempt over an interval, the size of the error is checked, to ensure reliable integration even over very long time spans. To determine the error each component of the local truncation error vector which is available at the end of the

integration interval is divided by the corresponding component in the scale vector. The largest component of the scaled error vector is finally determined and, depending on its magnitude, one of various options will be followed, as will be explained below.

The scaling factors of component j in the scaling vector $\underline{x}_{scale}$ is calculated as follows:

$$x_{j,scale} = \epsilon\left(\left|x_j(t=t)\right| + \left|H\frac{dx_j(t=t)}{dt}\right|\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(S-3)}$$

where $x_j(t=t)$ is the value of component j in $\underline{x}$ at the beginning of the time interval.

The scale vector is calculated at the beginning of every time interval (of length H), which is sent to the integrator, and is only recalculated within the interval if a discontinuity has been crossed. In essence the scaling factor of each component is a simple estimate of the value of the component at the end of the interval as the sum of the value at the beginning plus the expected change over the interval. This is multiplied by the user-specified accuracy ϵ.

The problem of this method of determining the scaling vector, is that it exaggerates the discontinuities: If at the beginning of the interval a component of $\underline{x}$ and its derivative are equal to zero, the scaling factor will be zero. To prevent the program from crashing, all scaling factors equal to zero are reassigned a very small value: Tiny = 10^{-30}. If the variable changes its value from zero within the interval, the division by the scaling factor will make the error estimate very large.

The decision of whether an error is too large or acceptable is taken by comparing it to a cut-off value Big. Here Big is a single user-specified variable and should be chosen with care: The larger Big is chosen, the less sensitive the discontinuity triggering will be. If an error is larger than Big, a discontinuity is anticipated and the simulator will change over to a special discontinuity handling routine. If the error is smaller than Big but larger than one, the integration over the interval is repeated, using a larger number of sub-intervals. Only when the error has been reduced to below 1, is the result of the integration over an interval accepted and integration of the next interval can proceed.

3.5 THE PROGRAM

The simulator package was written in the UNIX version of Fortran-77, with a printout available in Appendix I. A short description of the program follows, in which important details will be highlighted, followed by descriptions of the individual subroutines.

3.5.1 Organization of the State and Algebraic Variable Vectors

In a commercial simulator package any recompilation of code after changes in flowsheet design is highly undesirable. To prevent such recompilation, enough space should be available in the state and algebraic vectors to accommodate a certain maximum number of units with their connecting streams and connections, occupied by a certain maximum number of components.

Under normal circumstances, it is unlikely that all units, streams and connections will be used all the time with the maximum number of components. To prevent holes within the state and algebraic variable vectors, it is necessary to keep track of exactly how many variables are involved and to shift these as close to the front of the vectors as possible.

In the present simulator, this was achieved by using an index for each of the two variable vectors, which 'remember' where the variables associated with a specific unit, stream or connection are to be found within the vectors. These indexes are organised as follows:

INX(1) = 0

INX(i) = (no. of components)·(i-1)

ie. the index for unit i is always given as the position before the first of its variables. This makes it convenient to retrieve any variable, eg. component j in unit i is given by X(INX(i)+j). In other words each component is represented by the index position of its unit plus its own number in the sequence of the components.

The algebraic vector index, INA, is organised similarly, except that it contains an index for each unit, each stream and each connection, whereas the state variable vector contains information on the units only. For instance the derived variable j in unit i (eg. the volume

of unit i) is found at A(INA(i)+j). If we want the position of component j in stream i, this will be found at A(INA(i + total no. of units)+j).

This method of indices allows easy access to all variables by the procedures that have 'knowledge' of the plant layout and process. On the other hand, procedures that do not need to know about the flowsheet details (such as the integration routines) are simply presented with the vectors of the state variable and their derivatives, without needing to consider where each is to be found or what it signifies.

3.5.2 Main Program

The main program first reads in the flowsheet information from a data file and sets up the data structure accordingly. It then reads in data on the physical and chemical properties of the components involved. After asking for various decisions regarding the simulation details (via its subroutine: OPTIONS), it coordinates the simulation by allowing the integrator to calculate results in one minute (simulation time) steps. This will later allow the simulator to interface with a controller which gives control directives in discrete time intervals.

Plant data such as flowrates, densities, carbon transfers etc. was recorded in data files at ten minute intervals. The data is read in by the main program and is passed on to the integrator. Carbon transfer information (for schemes other than the plant recorded one) is also generated within the main program.

At specified time intervals, the simulation results are stored in data files for later retrieval and processing (this is done by the subroutine: WRITE).

3.5.3 Integration Package

ODEINT is the coordinating procedure or driver of the simulator. It divides the time interval from the main program into smaller parts and sends these to the integrating procedure. If a discontinuity is suspected, the discontinuity-handling procedure is called.

The actual integration is performed by the Bulirsch-Stoer integrator BSSTEP. From here the modified-midpoint routine MMID is called, which estimates the value of the state variables at the end of a time interval using the number of substeps given by BSSTEP. The results are passed to the extrapolation routine RZEXTR, which performs the Richardson extrapolation on the new vector using previous estimates if these are available. The extrapolated values are checked for their errors.

If the error is very large, a discontinuity is suspected and the whole time interval is passed back to ODEINT.
If the error is not so large, but also not satisfactory, MMID is called again with a larger number of subintervals, followed by another extrapolation. If the error at the maximum number of subintervals is still too large, the interval is decreased, and the integration is re-attempted.
If the integration has succeeded, a suggested new step size is calculated, which is passed back to ODEINT (see section 3.4.3).

The discontinuity handling routine PASS_DISCONT is called only when a discontinuity is suspected (refer to section 3.4.5 to see how that happens). It uses an interval-halving method to narrow down on the discontinuity and determines its order, by considering the sequence of successful and unsuccessful integration attempts and their associated divided differences. Based on the order of the discontinuity a minimum step-size is calculated, which will give an acceptable error if the discontinuity is crossed. The error associated with every successful step is also monitored, and if it is not acceptable, will be repeated, by passing it to BSSTEP via a special driver routine DRIVER2. Normally the integration will be done by either the modified-midpoint method in MMID (see section 3.4.1), or otherwise by a four-step Runge-Kutta method in RK4.
After the discontinuity has been passed, the remaining interval is passed back to ODEINT, which passes it to BSSTEP to restart the integration.

3.5.4 Algebraic Variable Routines

Before the derivatives of the state variables can been calculated, all algebraic variables

must first be calculated. To be able to calculate these variables, information on the particular process units and their interconnecting streams and connections is required. The calculations depend on the specific hydrodynamics and conditions of each unit and must therefore be performed by specialised procedures.

3.5.4.1 Algebraic Variables of the Units Only two algebraic variables are calculated for each unit in the subroutine ALGU. These are the mol total and the volume. They are calculated by simply summing the individual molar amounts or the individual molar amounts multiplied by the respective molar volume.

3.5.4.2 Feed Streams The algebraic variables associated with feed streams are calculated in the routine ALGS1 (as these are the Streams leaving the feed units which are assigned the defining number 1). The calculations depend on the specific feed unit, the amount of information available on it and the simulation options that have been chosen.

The most complex calculations are required for the pulp feed, especially when the data recorded on the plant is to be used. This requires the total volume of the stream to be adapted to the recorded volume flowrate, taking into consideration the individual volume fractions and also the recorded density which changes the relative amounts of solids and liquids.

For the other feed streams, the individual amounts can either be taken as equivalent to the variables in the associated feed unit or they can be scaled in proportion to the recorded flowrate of that particular stream or according to the flowrate of feed pulp.

3.5.4.3 Mixed Streams In the present setup on the simulated plant the stream coming from the pre-leach storage tank is mixed with cyanide and spent eluate in a distribution box, from where the combined exit stream is fed to the first leach tank. The distributor box has no holdup (ie. the pulp spends a negligibly short time in the box) so that it is not necessary to keep track of the state variables in the distributor box. The exit stream from this unit is therefore the sum of all the streams entering the box, as calculated by the routine ALGS3.

3.5.4.4 Screened Streams In more or less the opposite procedure to that employed by the last routine, ALGS4 separates the components of a single stream into two separate streams, according to the nature of these components. For instance a screen is employed to separate the coarse carbon and all its associated adsorbed species from the rest of the pulp. Again the screen has no holdup and the two exit streams are calculated directly from the incoming stream.

3.5.4.5 Transformed Streams To save space the variables monitored in different sections of the plant need not be identical. For instance all the carbon and associated capacity variables are of no interest in the leaching section and are therefore not included in the list of available components in the leach. Instead, a 'magic box' has been included at the transition between the two sections of the plant. This maps those variables in the leach, which are also of interest in the CIP, onto their new positions in the algebraic vector. Again this 'magic box' has no holdup and the exit stream can be calculated directly from the incoming stream (ALGS8).

3.5.4.6 Pre-leach Stream Unlike the streams before, this stream originates in a unit with holdup and therefore it is dependent on the hydrodynamics of that unit. The main function of the tank as it is at present, is to aerate the pulp and possibly to act as a buffer for the fluctuations in flowrate from the thickeners. Any extra lime needed to stabilise the pH in the leach would be added here as well.

The hydrodynamics of the pre-leach tank have been written as if the tank overflows into the distributor box. This is a reasonable assumption even though the exit stream is in reality controlled by a variable speed pump, as the level is controlled so tightly, that the effect is exactly as if the tank had just overflowed. The buffering capacity is therefore minimal.

The individual component flowrates out of the tank are calculated using the volume fractions of the components in the tank, making the assumption that the tank is perfectly mixed. All dissolved species are assumed to have negligible volume and flow out in molar proportion to the amount of water flowing out.

3.5.4.7 Leach Streams The stream out of one of the first nine leach pachucas depends not only on the level within the tank from which it leaves, but is rather dependent on the interaction of the levels in its tanks of origin and destination (refer to section 3.3.1.4). Only the stream leaving the last tank is calculated as a simple overflow from the tank.

Once the flowrate of the stream has been calculated (ALGS6), the individual component flows are calculated using their volume fractions in the unit, again assuming that the contents are perfectly mixed. The dissolved species do not contribute to the volume and their flow out is proportional (on a molar basis) to that of water.

3.5.4.8 CIP Streams During normal operation the calculations performed in ALGS7 of the streams leaving the CIP tanks are fairly simple. Each tank overflows independently and the pulp stream volume is thus a function of the volume in the tank. (Refer to the theoretical section on CIP hydrodynamics in Section 3.3.2.4 for a more detailed explanation of points raised here.)

The important difference between these streams and the other exit streams is that even though the contents of the tank are assumed to be perfectly mixed, the pulp stream does not contain any coarse carbon or any of the associated adsorbed species. (The only exception occurs if the leaking of carbon through the screens is being simulated.) In contrast, the fine carbon and its adsorbed species flow along with the pulp. The relative amount of fine carbon leaving the tank depends on its volume fraction in the tank (ignoring the volume occupied by the coarse carbon). The adsorbed species on fine carbon do not contribute to the volume and flow out in proportion to the amount of fine carbon just as the dissolved species flow out in proportion to the water.

When the transfer streams are turned on the hydrodynamics change. The transfer stream leaving a tank is calculated first. It contains all constituents in their volumetric proportions (molar proportions for dissolved and adsorbed species), with the total volume prespecified according to the simulation options chosen.

The pulp stream leaving the same tank must be influenced by the transfer of pulp from

it. Therefore its volumetric flowrate is determined from the volume in the tank as before, but the volume flowrate of the transfer stream is subtracted, to ensure that the total amount of pulp leaving the tank is not too large. Only then are the individual component flows calculated, taking into account the volume (or molar) fraction as was explained above.

Another condition requires consideration of how the streams leaving a tank are affected by screen blockages in the tank under consideration or the adjacent tanks. The transfer streams into and out of a tank with a blocked screen are stopped immediately. Pulp continues pouring into the tank, but the exit pulp stream is stopped so that the tank continues filling. When the screen unblocks, the exit valve is opened and pulp containing coarse carbon is carried downstream. The feed stream to the tank is stopped to allow the pressures above and below the carbon screen to equalize. Normal operation resumes only after unblocking and equalisation. (Refer back to section 3.3.2.4 for a further explanation.)

3.5.5 Derivative Routines

After all algebraic variables have been calculated, the derivatives of the state variables are determined.

The DERIVS subroutine is the supervisor routine for calculations of the derivatives vector. It first calls the relevant algebraic routines and makes sure that all algebraic variables have been calculated, before calling the derivative routines. A maximum of four cycles of algebraic calculations are permitted, before the program is aborted with an error message (refer to 3.2 for an explanation of why this is necessary). The derivatives are all calculated together without problem.

3.5.5.1 Unit Routines Derivatives are only calculated for units with holdup as these units have state variables associated with them. This section therefore excludes the distributor box, the screen and the 'magic box' which were discussed in sections 3.5.4.3, 3.5.4.4 and 3.5.4.5 respectively.

The state variables in the feed units do not change and therefore their derivatives are immediately set to zero.
In contrast, sink units can be used to monitor production and efficiency of the plant. By definition they have no exit stream. They are fictional units but can be imagined as very large tanks collecting all products leaving the plant. The state variables in sink units are updated by calculating their derivatives (in DIV2) from the information available for the product streams.

The three other types of units for which the derivatives are calculated are the reaction vessels. Streams flow in and out of the reactors and chemical reactions proceed between the various components within the unit. The extents of reactions could have been calculated as algebraic variables associated with the units, but it is easier and less memory-consuming to calculate them as temporary variables before the derivatives are calculated. The reactions which are incorporated have been mentioned earlier (for pre-leach and leach in 3.3.1.3 and for CIP in 3.3.2.3).

The derivatives are calculated by summing up all inflows, outflows and amounts produced or used up (according to the mol balances listed in equations L-18 and C-14).

3.6 COMPARISON WITH OTHER PROCESS MODELS

Steady-state models are useful to determine how the performance of a plant will be affected by a constant disturbance. Sophisticated commercial simulators have become available in the past few years and are used extensively when new processes are designed.

The first steady-state adsorption simulation was written by Fleming et.al. (1980). They assumed that carbon transfers along the cascade are continuous and equal. The same approach was used by Fleming et.al.(1983). In contrast Menne (1982) and Nicol et.al. (1984 a,b) used periodic movement of (part or all of) the carbon and assumed steady-state for the solution concentrations between transfers. The problem was that the loading of gold on carbon was time dependent and could not satisfactorily be modelled by any steady-state approach. The simulations of Nicol et.al. therefore became semi-dynamic to

take into account the pseudo or cyclic steady-state between transfers.

Similarly van Deventer applied his model (discussed in section 3.3.1.3) in a dynamic simulation of adsorption in a cascade of contactors (van Deventer,1984c; van Deventer, 1986a) but assumed that time occupied by transfers was negligible with respect to total time. Another application of this model was the simulation of a packed bed (Jansen van Rensburg and van Deventer,1985) where again no carbon was moved. This was extended to a packed column (van Deventer and Jansen van Rensburg,1987) which allowed only instantaneous carbon transfers to be made.

Glasser and Williams (1985) used Dixon's rate equation in applications to a column and a perfectly mixed continuous stirred tank reactor (CSTR) with either continuous or instantaneous transfers. Johns (1986) used essentially the same transfer schemes as Glasser and Williams, but used different adsorption rate equations.

The first dynamic simulation of the adsorption process which took into account movements of the pertinent reagents through the plant was presented by Carrier et.al.(1987) for a cascade of CSTRs. They wrote detailed mass balances for the ore, solution and carbon in each tank, allowing for sequential transfers starting at the top of the cascade and proceeding down the cascade as each transfer is completed. The model was kept very simple, using very few variables and simulating only the adsorption of gold from a gold-cyanide solution. Their assumptions included : no leaching in the CIP; attrition and poisoning of the carbon are negligible.

Stange and King (1987a) used a population balance approach to write mass balances for carbon particles with a range of sizes and a range of loadings. Various transfer schemes were possible. In this first paper they made a few simplifying assumptions (no carbon breakage, no leaching in the adsorption section and finally only one size class of carbon). The distribution of loadings is very cumbersome and in a second paper Stange and King (1987b) used the method of moments to solve the equations. In another paper on the subject (Stange et.al.,1990) a range of carbon sizes was used. The loading distribution was approximated by the average loading, which is permissable as long as the loading rate

equation is linear with respect to the loading term. Attrition, and hence the movement of carbon from one size class to the other, were still not considered.

In contrast to all previous models the importance of using plant data to describe the constantly changing concentrations, flowrates and hence rates was considered in this study. The influence of a badly controlled leach was considered significant enough for the whole leaching section to be included in the model. The hydrodynamics of all units, various side reactions, process disturbances (such as overflows, leakage and attrition of carbon) and process upsets were also included with the intention of creating a more realistic simulation than was previously possible. Such a realistic simulation does not only give insight into what happens during 'abnormal' operation, but is also vital in the development and testing of a control strategy for any real plant.

CHAPTER 4

SIMULATION RESULTS AND DISCUSSION

The simulator is based on an idealised version of a particular South African gold plant. It is able to approximate the true behaviour of the plant and can consequently be used to give insight into the effect of individual variables on the efficiencies of the plant sections being simulated. In trying to keep the simulator as simple as possible, only the most important factors influencing the efficiencies were taken into account. Others which did not change much under normal plant operating conditions were either not included as variables or were kept constant. Factors which fall into this category include the temperature of the pulp, the rate of agitation, air-addition rate, the fineness of grind, the type of ore etc. A lot of scope therefore exists to investigate the effects of these factors and to allow for them in the simulator at a later stage.

This report is restricted to those variables which were expected to be relevant and for which enough information was available, either in the literature or from plant samples, so that an approximate model could be formulated.

It is again convenient to look at the two sections of the plant separately. They do obviously form a whole as far as plant efficiency studies are concerned, but they are so different and affected by such different variables, that is easiest to treat them as merely connected but totally individual processes. Each can then be evaluated according to its own efficiency and hence improvements for each can be suggested separately.

4.1 THE LEACH

This section is mainly concerned with the leaching of gold from the ore and its efficiency is of prime interest. Any other process taking place is only significant in the degree to

which it hinders or improves the leaching process.

As a result the reactions chosen to represent the leaching process (as outlined in 3.3.1.3 above) contain only few variables. The variables, besides gold, which are involved in the leaching reaction are the concentrations of oxygen and cyanide. They are the critical variables in the leaching process and are therefore included in various side reactions as well. The side reactions consume these often costly reagents without producing an economically useful product. They are included in the simulation as they play an important role in determining the profitability of the plant.

By looking at Table II, one can see that these are not the only species included in the leach simulation. Water and the rock material (represented by SiO_2) provide most of the bulk, even though they are hardly affected by the reactions. They have to be included to make the hydrodynamics in the leach more realistic. The dissolution of lime was included to make it possible for the pH to be changed dynamically. At present the pH is not used in the rate reactions as the pH control on the plant was good (it was nearly constant at 10) and information on the effect of changes in pH on the rate of leaching was thus not available for this particular case. In general, the loss of cyanide and the leaching reactions are dependent on the concentration of OH^-. If the simulator is therefore to be applied to another gold plant, in which the pH fluctuates enough for its effect to be measurable, the affected reaction rates can and would be made a function of the OH^- concentration.

All those factors which are known to affect the leach and for which enough information was available were therefore investigated. These are: the effect of oxygen addition, the effect of cyanide addition, the effect of flowrate variations and the effect of spent eluate addition. The results of all the simulation runs are summarized in Table IV below.

Simulation Description	Efficiency (%)	Average Discard Gold Grade (mg/t)
Constant Feed, Constant Cyanide	99,594	45,7
No O_2 in Leach Feed	99,554	50,2
Lower Equilibrium Dissolved O_2 Conc.	99,175	92,9
1 hr Cut in CN^- Addition	99,592	46,0
Plant Feed Q and ρ. Const. CN^- Addition	99,554	50,2
Plant Feed Q and ρ. Prop. CN^- Addition	99,558	49,8
Plant Feed Q and ρ. Plant CN^- Addition	99,236	86,1
Plant Feed Q and ρ. Plant CN^- and Spent Eluate Addition	99,372	70,7

Table IV : Leach Simulation Results

The leach efficiency is calculated as

$$Efficiency = \frac{(G_{Au,f,in} + G_{Au,s,in}) - (G_{Au,f,out} + G_{Au,s,out})}{G_{Au,f,in} + G_{Au,s,in}} .100 \quad \text{.....(L-29)}$$

where $G_{Au,f,in}$ and $G_{Au,s,in}$ are the grades of fast and slow leaching gold in the feed ore, and $G_{Au,f,out}$ and $G_{Au,s,out}$ are the corresponding grades in the ore leaving the leach. (grades are calculated as the mass of valuables (g) per mass of total ore (t).)

The first week in all simulations allows the system to reach an approximate steady-state, with efficiency being evaluated over the second week. The efficiencies were not evaluated as instantaneous values. Instead, the amounts of gold entering and leaving the leach were summed over the whole second week giving an average efficiency over the week in each case. At true steady-state the numerator should be equal to the amount of dissolved gold which left the leach.

The fact that the leach efficiencies are all unusually high has two reasons:

- All leaching which in reality occurs in the leach and in the CIP is assumed to occur in the leaching section of the plant only. From the plant data it was evident

that most leaching does occur in the first five leach tanks but another significant amount of gold dissolves in the first CIP tank. The assumption of no leaching in the CIP was nevertheless made to allow separate evaluations of the leaching and adsorption efficiencies.

- While the dissolvable gold was divided into the fast and the slow leaching fractions, the undissolvable gold was ignored for the simulation. Undissolvable gold is usually assumed to be that fraction of the gold which is totally occluded by the gangue material and would only be liberated by finer milling or another physicochemical process such as roasting. The undissolvable gold usually constitutes about 2,5 % of the total gold entering the leach.

The true efficiencies would therefore lie substantially below the reported figures. The importance of the listed efficiencies therefore lies in their relative magnitudes rather than in the actual values.

4.1.1 Base Case

As described above the system in each investigation is initially empty and is allowed to fill up and approach steady state if this is possible. To make an objective evaluation of different simulation conditions easier, one reference case was chosen against which each of the others can then measured.

The reference or base case for the leach efficiency comparisons is the case for which all additions are smooth and nearly optimal. Initially the plant is completely empty, so that all state variables and their derivatives and all algebraic variables are zero. The pulp is added at a constant rate and density, with lime and cyanide additions in correct proportion to the flowrate of pulp. The concentration of dissolved oxygen in the pulp coming from the thickeners is constant and relatively high.

The dynamic changes of the gold concentration in the ore and in solution are shown in Figure 16 from the time when the plant is still empty until it has filled and reached an approximate steady state. As the pulp flows into the first pachuca (leach 1) it is mixed with cyanide. At the first moment when the first bit of pulp flows into the tank and

leaching has only just started (shown by the first vertical line on the left), the amount of solid gold is still high, but the gold dissolves very rapidly, reaching an equilibrium value of about 25 % of the feed concentration. This fast dissolution is mirrored by the sharp rise in the $Au(CN)_2^-$ concentration of the first tank, reaching its equilibrium at just above 0.04 $kmol.m^{-3}$.

The change in the amounts of solid and dissolved gold in the next two tanks (leach 2 and leach 3) is also shown: as pulp first flows into each tank (next two vertical lines) the gold grade is still the same as in the previous tank but in each tank the gold grade quickly decreases as the tank fills up. As can be seen from the graph for the last leach tank (leach 10) the amount leached in the last seven pachucas is very small, but not insignificant.

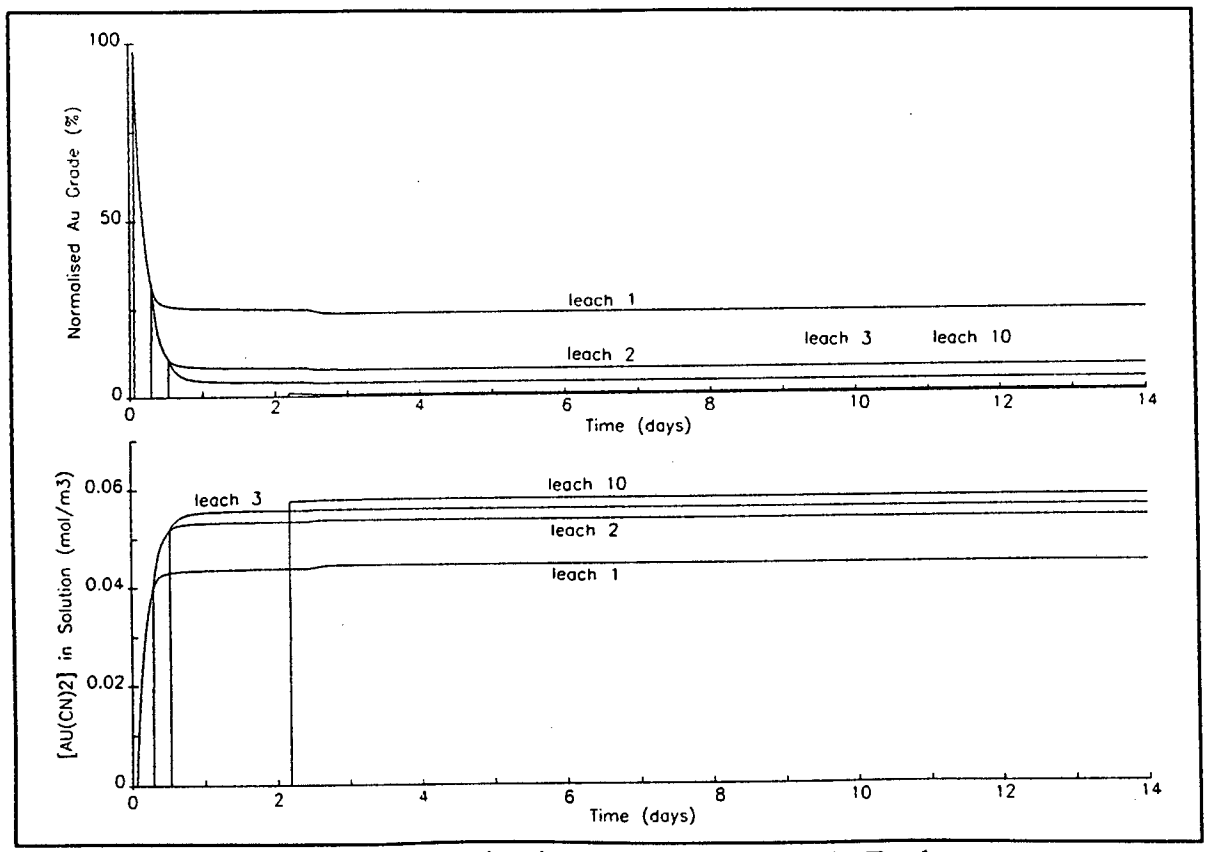


Figure 16 : Gold in Ore and Solution in the Leach for Steady Feed

In contrast, the relatively slow leaching rate of the competing metal species is shown by the more widely separated concentration lines in the first three pachucas (see Figure 17: leach1, leach2 and leach3), with the amount dissolving in each pachuca being roughly a third of the amount of metal entering.

As was explained before, the 'metal' species is an imaginary metal, which sums up the effect of all the competing metals. The competing metals (the most important of which are silver, copper, nickel and iron) behave quite differently and this method of summing up their effects was intended to make the modelling simpler. For instance silver occurs in very small amounts in the ore but leaches to near completion, while iron occurs in very large amounts but little of it actually leaches. Therefore only the dissolvable fractions of each of theses metals were added to represent the dissolvable fraction of 'metal', which was included in the model. The rate equation for 'metal' dissolution is also written to take only this dissolvable portion into account.

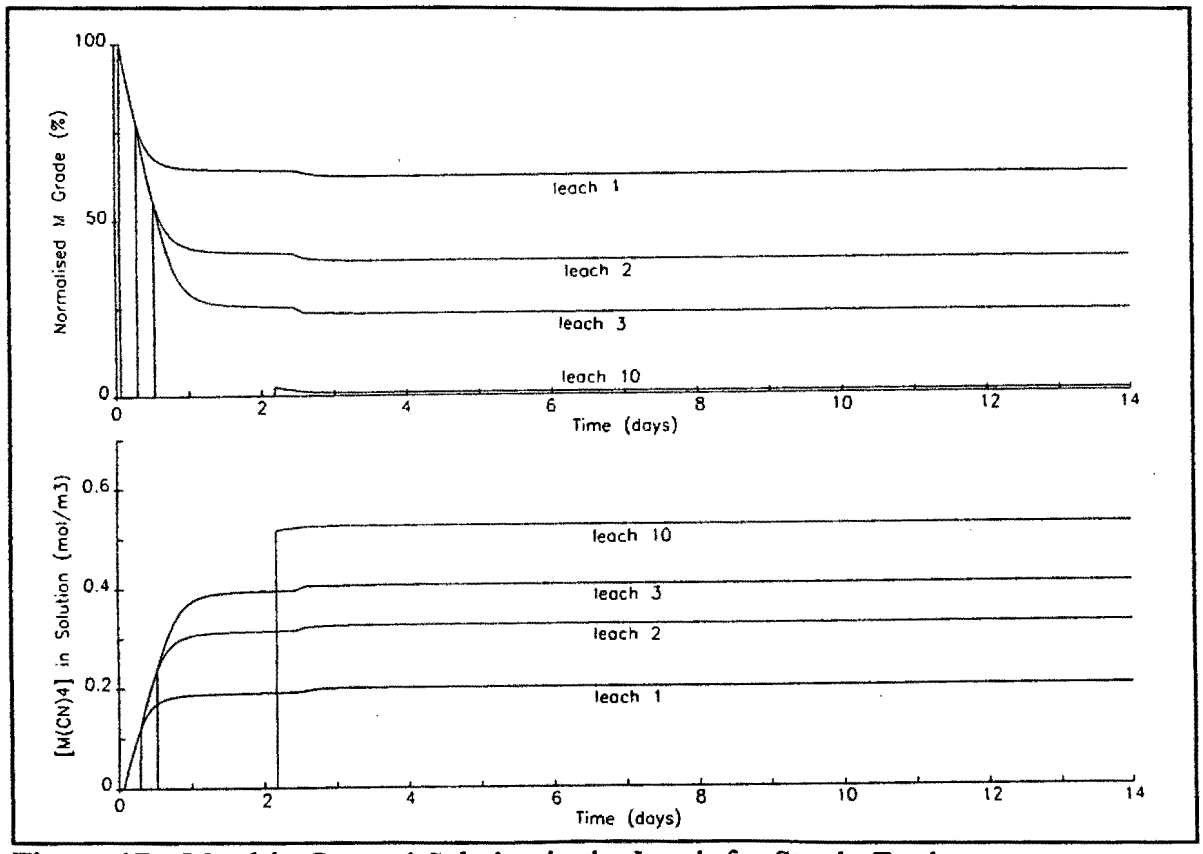


Figure 17 : Metal in Ore and Solution in the Leach for Steady Feed

The inclusion of the 'metal' species in the model was important as it accounts for the consumption of most of the cyanide and dissolved oxygen. This is partly an effect of the larger number of cyanide ions used in the formation of its complex partly caused by the greater amount which dissolves - the final concentration of metal-cyanide leaving the leach is about ten times of the gold-cyanide concentration (compare the solution concentrations for metal and gold cyanide in leach 10 in Figure 17 and Figure 16).

The change of dissolved oxygen concentration in the leach cascade as a function of time is shown in Figure 18. Note how the concentrations of dissolved oxygen in the early part of the week are still changing before reaching equilibrium. The concentration in the pre-leach tank (feed) rises steadily until it reaches its equilibrium at just above 0,2 $mol.m^{-3}$. In contrast, the dissolved oxygen level in the pulp flowing into the first leach pachuca initially is the same as that in the pre-leach tank (the vertical line closest to the vertical axis reaches the feed curve). The pulp has already been mixed with cyanide and as the reaction starts in this first pachuca, the dissolved oxygen level drops. It recovers slightly as the concentration in the pulp from the pre-leach tank increases and the initial rate of reaction slows down so that it finally reaches an equilibrium of approximately 0,18 $mol.m^{-3}$. As each of the later tanks fill, the concentration of dissolved oxygen rises further indicating that the rate of consumption has become less than the rate of dissolution.

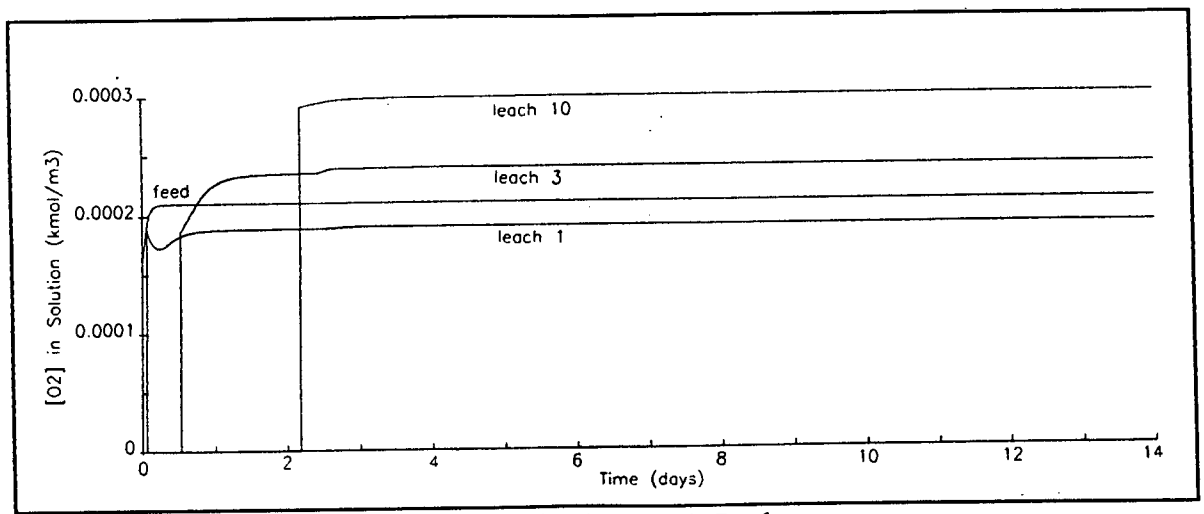


Figure 18 : Dissolved Oxygen Levels in the Leach Pachucas

The slight increase in the dissolved oxygen concentration in tank 3 on day 3 (also visible in Figure 16 and Figure 17) is a result of the hydrodynamics of the plant. Before this point, the pulp in each leach pachuca overflows into the next tank as soon as the level reaches the top of the weir in the particular tank. When the last tank fills, though, the pulp does not overflow at the same volume as the earlier tanks but at a slightly larger volume. As a result the levels in all the previous tanks start rising and begin to interact with each other. This increase in capacity of the tanks allows the dissolved oxygen levels to rise slightly further than before, giving the extra little bump in all the curves.

The efficiency of the base case was 99,594 %. All other efficiencies lie between 99 % and this value. As was explained on page 70, these efficiency figures are all artificially high because only the dissolvable fraction of gold is considered and the leaching reaction is restricted to the leaching section of the plant. It may therefore seem arbitrary to compare numbers which are so similar, but if one considers the amount of gold passing through the plant, an improvement of only 0,1 % represents an increase in production of nearly a third of a kilogram of gold per week. At a value of R30 000.kg^{-1} this represents an increased return of R10 000 per week.

4.1.2 Effect of Oxygen

The particular plant studied does not have a problem with dissolved oxygen concentrations. This is partly a result of the pre-aeration of the pulp before it enters the leach pachucas. Another reason is that the air in the pachucas is added within the downdraught tubes (refer to Figure 8). This not only ensures a long contact time of the air with the pulp, but also, because the pachucas are so deep (19 m), the pressure at the bottom of the tank causes oxygen to dissolve to supersaturation.

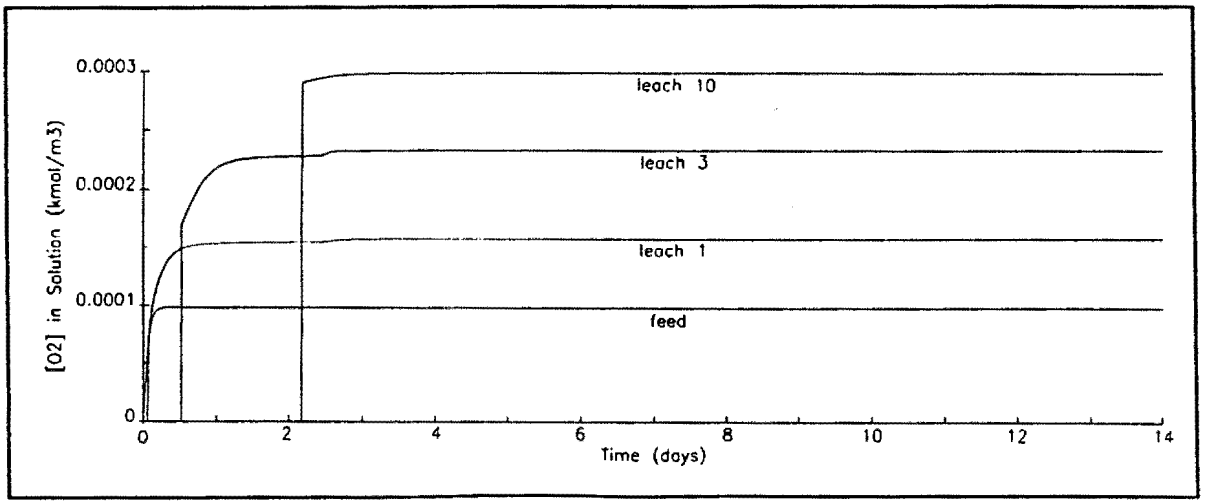


Figure 19 : Dissolved Oxygen Concentrations in the Leach without Pre-aeration

To see what the effect of pre-aeration is, a simulation was run with no air being added to the pre-leach tank. The resulting oxygen curves are shown in Figure 19. While the dissolved oxygen levels are significantly lower in the first tank for this simulation than those shown in the corresponding graphs in Figure 18, the steady state value in the last

tank is only marginally lower than before. If one remembers that normally about 80 % of all leaching occurs in the first leach tank, it is not surprising, that the efficiency of the leach has dropped to 99,554 %. The pre-aeration of the pulp alone therefore ensures an increase of gold dissolution of nearly 0,15 kg of gold a week.

Weichselbaum et.al.(1989) report that at normal atmospheric pressure at 1800 m above sea level, the equilibrium concentration of oxygen in pulp is 7,4 $mg.l^{-1}$, which is equivalent to 0,231 $mmol.l^{-1}$. This is the concentration which would be achieved if the air were not carried right to the bottom of the tank but if it were introduced outside the downdraught tubes instead (refer to Figure 8 again). In that case - if it can be assumed that the agitation is as vigorous as before and oxygen therefore dissolves at the same rate as before - the leach efficiency is reduced to 99,175 % ! This lends credibility to the various attempts to improve leaching performances by adding more oxygen, as described by Arnold and Stephens (1988) and by Rodrigues (1990).

4.1.3 Effect of Cyanide

Cyanide is consumed very quickly in the pulp. Because of a lack of suitable instruments, the concentration of cyanide is impossible to control accurately, regardless of whether control is automatic or manual. To prevent any loss of gold due to the lack of cyanide, it is usually added to the leach pulps in great excess. This implies that the concentration of cyanide is not rate limiting, and a strong dependence such as on the concentration of dissolved oxygen is not to be expected. (Remember the form of rate equation of gold dissolution, L-20, incorporates this switch-over of rate dependence from control by cyanide to control by oxygen. As long as the concentration of cyanide is more than 6,6 times that of oxygen, the concentration of oxygen will be rate limiting.)

The effect of cutting the cyanide addition for one hour caused a noticeable drop in the concentration of cyanide in the first tank, mirrored by a marked rise in the undissolved gold. This is smoothed out, though, as the pulp proceeds through the other nine leach pachucas, and overall this causes an increased loss of gold of only 5,5 g.

The simulations above were run with a cyanide addition of 0,25 mol.s^{-1}. When the addition rate is increased to 0,32 mol.s^{-1} (an increase of 28 %) the concentration in the first leach tank increases from 5,5 mmol.l^{-1} (143 ppm CN^-) to 7,2 mmol.l^{-1} (187 ppm CN^-) which is not an unusual concentration for leach pulps. The gold dissolution efficiency increased by 0.061% to 99,655%. This shows that excessive cyanide additions do have a beneficial effect in forcing the reaction towards the products, but this effect becomes less pronounced the higher the cyanide concentration. At some stage an economic cut-off point will be reached where the cyanide added will cost more than the extra amount of dissolved gold is worth.

The risks involved in working at such high cyanide levels should also not be forgotten. In the production of gold it can be detrimental, by for instance passivating the surface of the gold by the formation of an insoluble AuCN layer (Fink and Putnam, 1950). This is usually prevented by the natural occurrence of lead and other metal salts in the ore, though. The adsorption of cyanide later in the CIP is detrimental to the adsorption of gold and the loss of cyanide by hydrolysis presents acute danger for employees on the plant. The dumping of cyanide containing pulps underground or on dumps also presents a health risk to those exposed to the cyanide.

Another simulation was run using the addition intervals as recorded on the plant. This is discussed later in Section 4.1.5.

4.1.4 Effect of Flowrate

Data logged on the same gold plant as was simulated in this project was available for testing the effect of changing flowrates on the leach efficiency.

With expansion plans in mind, the leach pachucas were chosen with very large volumes. The residence time of the pulp in the leach cascade is of the order of two and a half days, which is unusually long for such an operation. Also, as was explained before (section 3.3.1.4), the pachucas are built in such a way that the levels can vary over about 3 m in all ten tanks. This gives the leach train enormous buffering capacity of nearly 2000 m^3 or

about 10 hr at normal pulp flowrate.

At the same time the feed to the leach fluctuates considerably (see Figure 20) and a fairly obvious question is whether the buffering capacity is enough to ensure a maintained leaching efficiency. A simulation was therefore run with plant data on feed flowrate and density as shown in Figure 20. Cyanide addition was kept proportional to the feed flowrate. The feed flowrate was scaled in such a way that the average flowrate of the week was the same as the constant flowrate used before. The effect of the changes in density was such, though, that relatively more solids, and hence more gold, were added in the week than before.

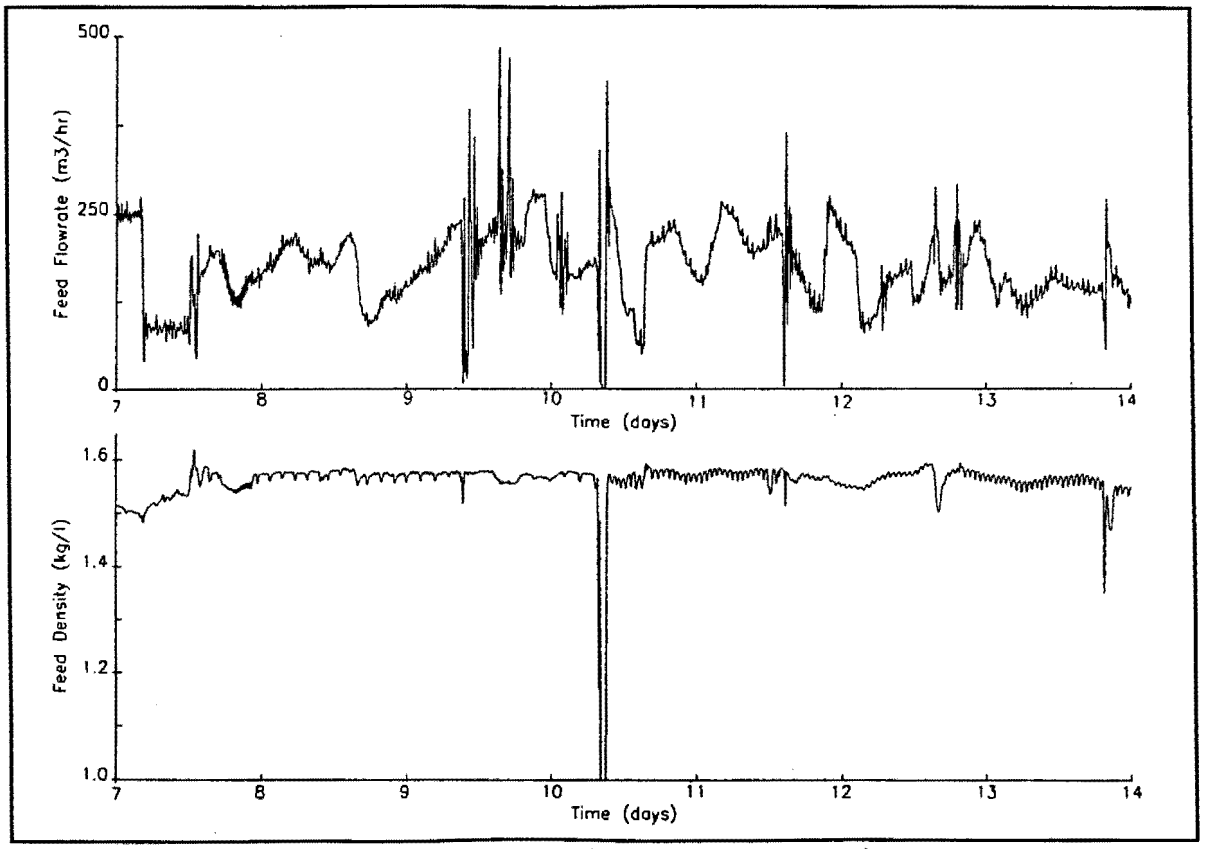


Figure 20 : Flowrate and Density Fluctuations in the Feed to the Leach

The total effect of these conditions was to reduce the efficiency of the leach to 99,558%. The extra amount of gold which was not dissolved as a result of the fluctuations amounted to nearly 0,12 kg for the week.

4.1.5 Effect of Cyanide and Flowrate Combined

A simulation was also run in which the cyanide addition was kept constant instead of being proportional to the fluctuating pulp flowrate. This was done to see whether the inclusion of a proportional controller would pay for itself instead of adding a constant amount of cyanide. The efficiency in this case was actually not much lower : 99,554 % as compared to the 99,558 % reported above for constant cyanide addition. The small difference is a result of scaling the magnitude of the pulp flowrate in the previous section, which ensures that the average of the variable feed flowrate over the week is equal to the constant flowrate used before. Had the flowrate not been scaled and the long-term average flowrate been higher, the efficiency would have suffered more with constant cyanide addition. If, on the other hand, the long-term average flowrate had been lower, more cyanide would have been wasted with only a small increase in associated efficiency. A proportional controller is therefore highly desirable, even if the results above do not necessarily indicate that.

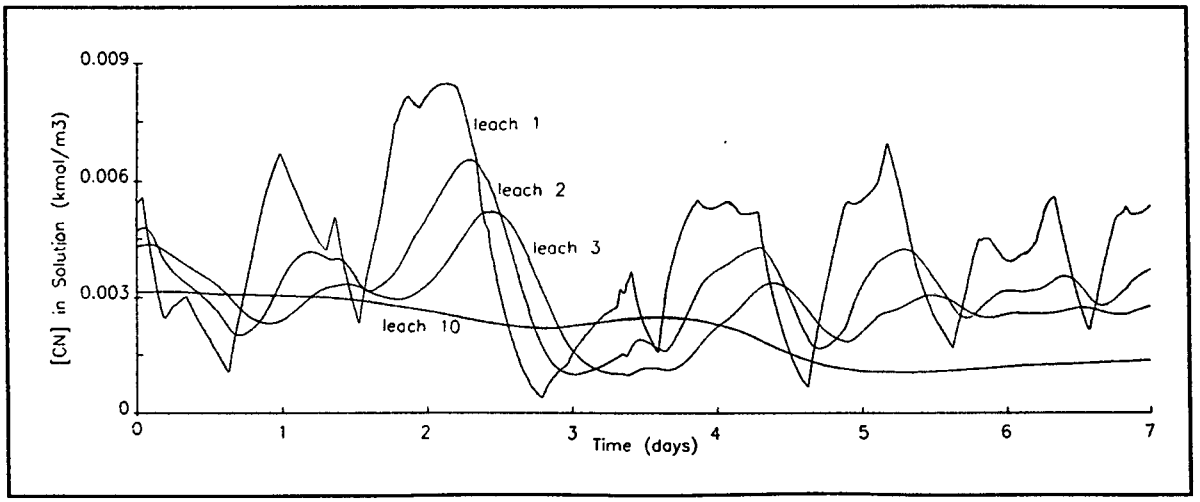


Figure 21 : Cyanide Concentrations in the Leach with Random Cyanide Additions

In contrast to the controlled or constant addition of cyanide the addition on the plant is nearly random. Among the data which was collected, information on the addition of cyanide was also available. As with the feed pulp flowrate the flowrate of cyanide fluctuates greatly, and usually not even in approximate proportion to the pulp flowrate. As a result the concentration of cyanide in the pulp fluctuates dramatically as shown in Figure 21.

As may be expected, the effect of these large fluctuations is a relatively large drop in leaching efficiency over the week to 99,236 %. Again this may not seem too bad, as compared to the base case of 99,594 %, but the extra mass of dissolvable gold, which did not dissolve during this week alone had a mass of 1,19 kg, worth about R36 000 !

Any kind of control scheme, even a simple flow controller, would definitely improve the efficiency of the leach. In all likelihood such a controller would pay for itself in a matter of weeks.

4.1.6 Effect of Returned Eluate

Before one is tempted to attach too much significance to the above result, there is one very important effect which may not be overlooked, and that is the addition of spent eluate to the leach pulp. The eluate is extremely alkaline and also tends to contain large amounts of cyanide and will therefore have a balancing effect on the cyanide concentration.

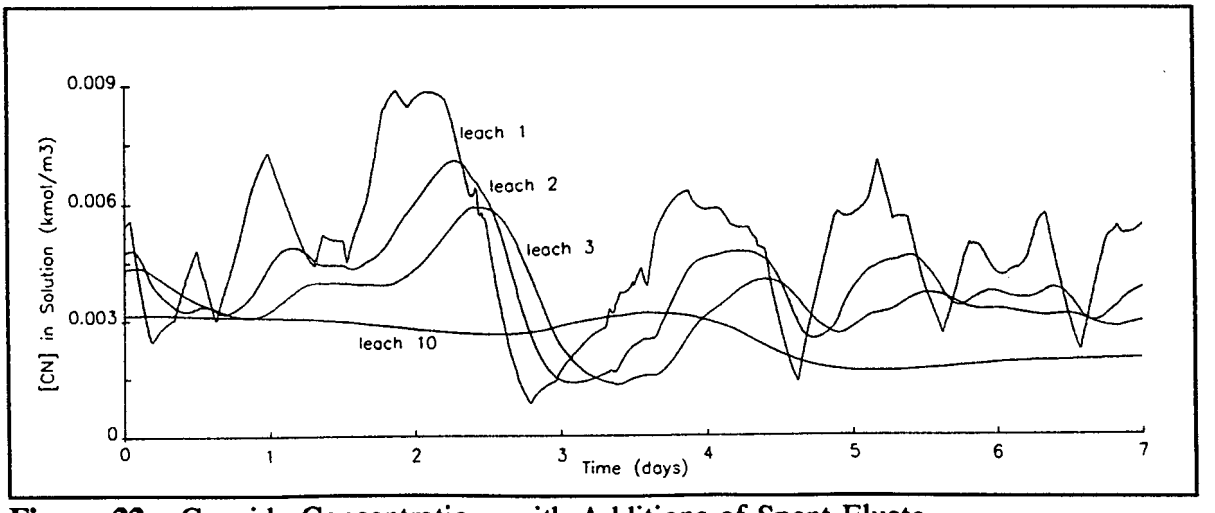


Figure 22 : Cyanide Concentrations with Additions of Spent Eluate

Information on the addition of spent eluate is available but despite the fact that the addition rate is variable, only an on/off signal was sent to the plant computer. This obviously makes it difficult to simulate the true concentration of cyanide during the time of data collection as neither the amount of spent eluate added nor its composition are known. The method used here was simply to assume that the eluate flowrate was of constant magnitude during the pumping intervals indicated by the data and to keep the

composition constant.

The situation as compared to the previous one is much improved (Figure 22) with an efficiency of 99,372%. This can explained by the method of operation of the plant: When spent eluate is to be pumped to the leach, the addition of cyanide is either reduced or cut completely. Therefore the periods of low cyanide concentration as portrayed earlier (Figure 21) are actually exaggerated. If more accurate information on the flowrate of spent eluate had been available, it might have been possible to show how returned eluate additions are planned into the cyanide housekeeping and that the cyanide concentrations never quite drop to the levels shown in Figure 21.

This shows what an important effect the controlled addition of the spent eluate has on the efficiency on the plant. Some kind of an intelligent control for total cyanide addition (including the spent eluate addition) is worth considering as the fluctuations in the cyanide levels are still excessive as shown in Figure 22. Such a control strategy would need to involve some reliable measure of cyanide concentration, but it is likely to pay for itself, even on a well maintained plant.

4.2 THE ADSORPTION SECTION

The factors which affect the adsorption efficiency most strongly are the concentration of the dissolved species in solution, the concentration of the adsorbed species on carbon and the carbon concentration. The two last factors are dependent on both the rate of pulp flow through the cascade and the scheme of carbon transfers. Other factors which have been included in the simulator include the attrition of carbon to fine particles which pass through the screens unhindered, the effect of leakage of large carbon particles through the screens and screen overflows.

As indicated in Table III (in section 3.3.2.1), water and gangue (SiO_2) are included in the species to provide the pulp with bulk volume which is necessary for the calculation of the hydrodynamics. While the concentration of OH^- is included as a separate state variable within each tank, the rate equations describing adsorption or the oxidation of cyanide were

not written in terms of pH. This was again the result of a lack of suitable information on how the pH affects these reactions because the pH in the adsorption cascade did not vary enough during the sampling campaign for a reliable dependence to be determined.

Similarly the desorption parts of the adsorption equations should be functions of all adsorbed species, which would be the only way of simulating competitive adsorption. The data available until now did not suffice to find suitable rate equations, but it would be very desirable to include competitive adsorption in any extension of the simulator.

As can be seen in section 3.3.2.3, the division of the coarse carbon into two fractions (one of which contains only micropores while the other contains only macropores) and by also considering the fine carbon as a separate adsorption medium, it means that three rate equations have to be written for each of the adsorbing species. Taking into account only the gold cyanide, the metal cyanide and the free cyanide ion this gives a total of nine adsorption rate equations (C-18a,b,c; C-19a,b,c and C-20a,b,c), each requiring its own adsorption term. This may seem very clumsy, but is essentially the simplest simplification possible of a distributed description of the adsorption system above the trivial case simulated in most previous attempts (section 2.2.5).

Table V below summarizes the results achieved in the various simulation runs carried out to test what the effect of the factors listed above will have on the efficiency of the adsorption cascade.

The efficiency is measured in terms of the total amount of gold adsorbed and transferred to the elution as compared to the total amount of dissolved gold which entered the adsorption section. Only the gold adsorbed on the coarse pieces of carbon can be retrieved, while the fine carbon is carried out of the bottom end of the cascade together with its adsorbed gold and is lost.

As in the case of the leach efficiency calculations, the efficiency is measured in terms of the summed amounts of gold in the various fractions over the duration of a second week, after the system was allowed to approach (cyclic) steady-state during the first week. The

problem with the cyclic nature of the steady state is that the efficiency depends on the time relative to a transfer that the efficiency is calculated: The efficiency is higher if it is calculated before a transfer than if it is calculated after the transfer. That is why the efficiencies listed in Table V are given to only 2 decimal places. The error in the second decimal place is significant, so that slight differences in the results may well be caused to the timing of the efficiency calculation rather than process changes.

Simulation Description	Efficiency (%)	Average Mass of C (kg)	Gold Holdup (kg)
No Attrition	99,99	5711	43,1
Simultaneous, 5000 kg/16 hr	97,99	5624	48,4
Simultaneous, 2500 kg/8 hr	98,09	5624	47,9
Continuous, 5000 kg/16 hr	98,08	5685	48,4
Continuous, 2500 kg/16 hr	97,78	5658	90,3
Consecutive, 5000 kg/16 hr	97,66	4294	31,9
Consecutive, 2500 kg/8 hr	98,07	5260	41,1
Carbon Leaking, no Top-ups	98,01	5505	46,7
Carbon leaking with Top-ups	97,97	5724	49,2
Top Heavy Carbon Profile	97,73	6667	62,5
Bottom Heavy Carbon Profile	98,11	6679	49,1
Regular Unequal Transfers	98,08	5711	52,3
Irregular Equal Transfers	96,62	3650	29,3
Plant Recorded Feed Flowrate	97,75	5686	54,4
Plant Recorded Transfers and Feed	96,15	5714	65,7
Screen Overflow (Ideal Case)	97,99	5603	47,8
Screen Overflow (Plant Data)	96,13	5718	67,0

Table V : CIP Simulation Results

4.2.1 Base Case

The case with which all others are compared represents an idealized version of existing plant conditions. The carbon profile is initially smooth and the carbon transfers are all started at the same time and have equal flowrates, so that the carbon profile is essentially never disturbed. The attrition of carbon causes a steady drop in the total mass of carbon in each tank (see Figure 23) as the carbon fines are not compensated for by the transfers.

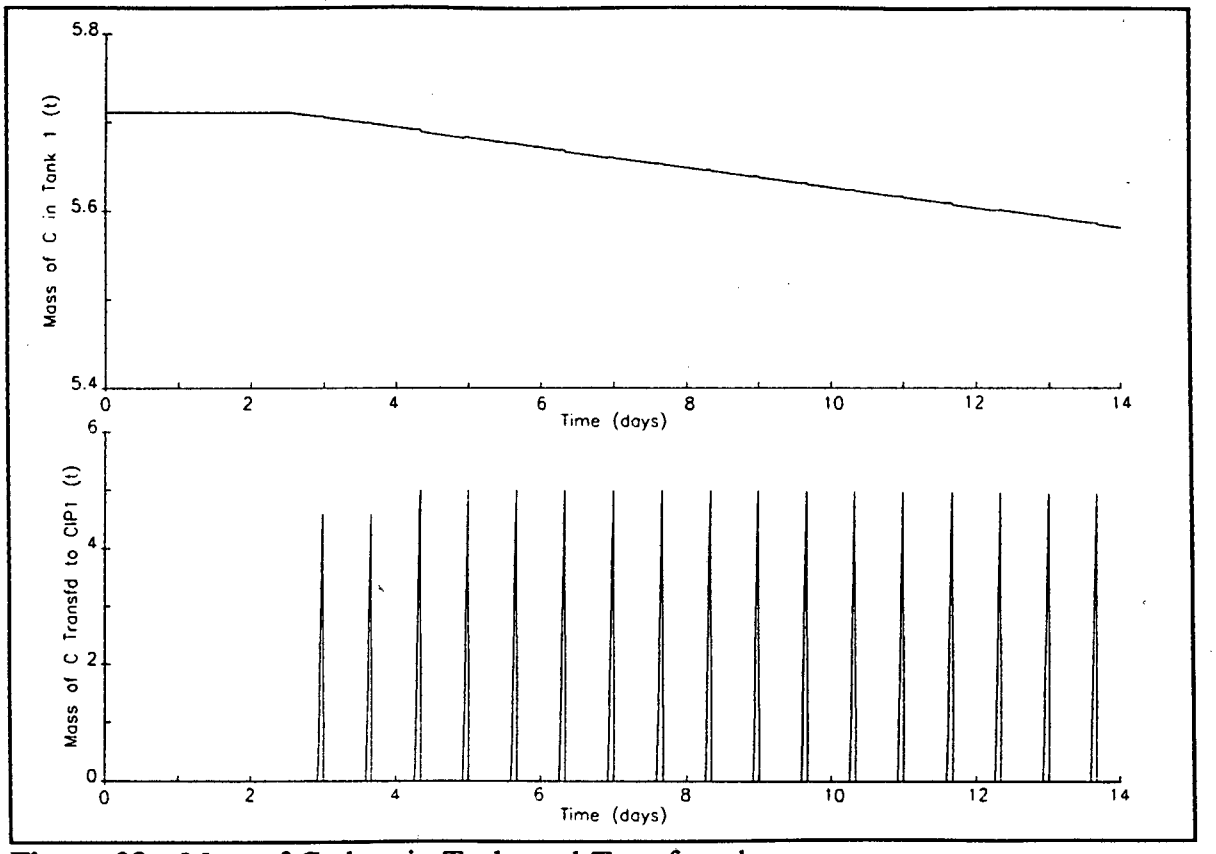


Figure 23 : Mass of Carbon in Tanks and Transferred

The plant target is to pump 7500 kg of loaded carbon to elution per day, and hence 7500 kg must be pumped from each tank to the one above. The mass of carbon in each tank is only about 5600 kg and therefore the transfers are limited to 5000 kg which are pumped in every second shift. This means that three transfers are carried out in two days, giving the desired throughput of 7500 kg per day. Pumping 5000 kg of a possible 5600 kg from each tank implies that transfers are nearly 'complete' - if one ignores the amount of carbon which short-circuits, and the tenth that is left behind (ie. the difference between the 5600 kg in the tank and the 5000 kg transferred).

The effect of the periodic transfers is, as can be expected, highly disruptive for the loading process. The profiles for the solution concentrations of gold-cyanide and the masses of adsorbed gold in each of the tanks are shown in Figure 24.

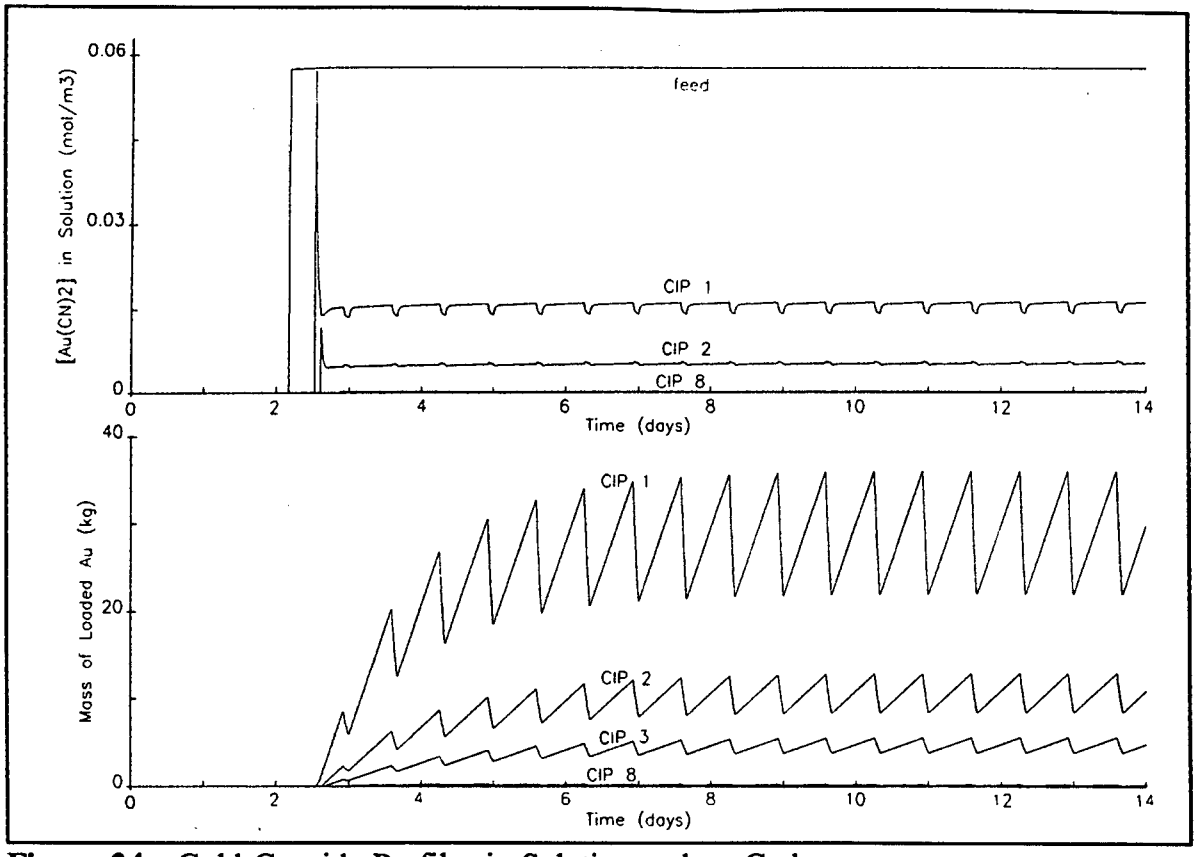


Figure 24 : Gold-Cyanide Profiles in Solution and on Carbon

As in the case of the leaching rate, the adsorption of $Au(CN)_2^-$ is also very rapid. The solution concentration in the first tank drops by more than two-thirds of its feed concentration. The equilibrium loading was found to be so high that all gold loadings under normal conditions lie far from equilibrium, making adsorption dependent on the solution concentration only. As a result the loading on carbon rises linearly between transfers, only to fall sharply when the transfer starts. As the carbon transferred from the lower tanks contains progressively more gold, the loading range (between peak and valley) rises and reaches an approximate pseudo-equilibrium after a week. A pseudo-equilibrium is evident in the similar shapes of successive saw-teeth in the graph. These show that the cascade has reached a state where successive loading cycles are identical, with the carbon always entering the stage with the same loading and always leaving at a specific higher loading.

The loading behaviour of metal-cyanide is different to that of gold-cyanide (Figure 25) in

that its maximum loading capacity is lower and is thus reached fairly quickly. In actual fact the maximum loading of the metal-cyanide is so low that the amount of metal-cyanide which can load is only roughly double as much the amount of gold-cyanide that is usually loaded and this despite the 10:1 ratio in their solution concentrations.

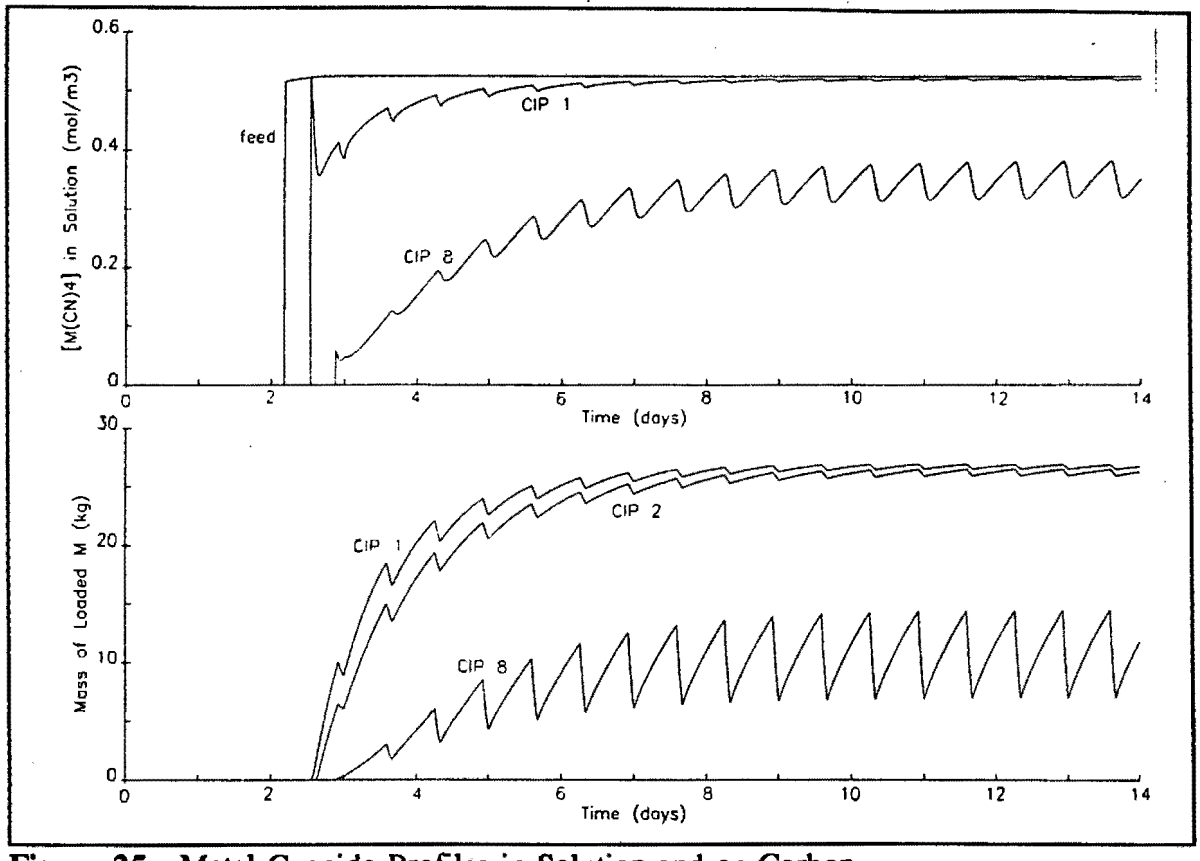


Figure 25 : Metal-Cyanide Profiles in Solution and on Carbon

Initially most metal-cyanide (like the aurocyanide) is adsorbed in the first few tanks, but it quickly reaches maximum loading. The effect is that the concentration of $M(CN)_4^{3-}$ in solution passing to the lower tanks is quite high. The metal-cyanide therefore starts to load to quite a significant degree on the carbon in these lower stages. As this more loaded carbon is transferred up the cascade, little additional metal-cyanide can be adsorbed. This then explains the shape of the metal-cyanide profiles at pseudo-equilibrium: Little loading occurs in the top tanks and therefore both the solution and loading profiles are bunched for these tanks. Lower down the cascade, where the fresh carbon still has a higher capacity, metal-cyanide is adsorbed and the profiles lie further apart.

The efficiency of this base case was calculated as 97,99 %. Other measures which were

recorded for all simulations for comparison purposes are the average mass of carbon in the cascade adsorbers (averaged over time and all tanks) and the total retrievable adsorbed gold in the cascade at any point in time (as an average over the week). The average mass of carbon in each tank during the week used as the base case was 5624 kg. The mass of retrievable gold locked in the cascade averaged 48,392 kg. Obviously this amount will be significantly higher just before a transfer and quite a bit lower afterwards.

4.2.2 Effect of Attrition

Attrition was included in the base case as it is inseparable from any application of activated carbon. Unlike carbon leakage for instance, it cannot be prevented. It is a natural process of degradation of the brittle carbon particles as they bump into each other and are scoured away by the abrasive particles of rock. Whyte et.al.(1990) noted that the rate of attrition is proportional to the concentration of carbon in a tank. Regardless of whether the concentration is low as in normal CIP tanks or as high as in the pump cell described by Whyte et.al., attrition is inevitable.

And yet it is necessary to determine what the effect of this attrition will be. One simulation was therefore run to see how much the base case would have been improved if no attrition had occurred. The conditions are exactly the same as those chosen for the base case : constant feed flowrate of constant composition with large (5000 kg) simultaneous transfers regularly started every 16 hr and all with equal flowrate.

As can be expected, when no attrition, leakage or overflows occur the mass of carbon in each tank remains constant throughout the operation. The effect on the efficiency was to increase it to a remarkable 99,99 % ! This shows what a detrimental effect attrition has and hence the limit in achievable improvement should be kept in mind when any optimisation of the CIP circuit is attempted.

The reasons why attrition affects the efficiency of the adsorption section so strongly are:

- Some gold is carried out the bottom of the cascade by being adsorbed on the fine carbon particles. The larger of these may be recovered by the Delkor screen,

through which the discard stream passes.

- The more important effect of the fine carbon is the way in which it changes the solution profiles. The gold-cyanide ions load onto the fine carbon particles very quickly because of the small particle sizes. As a result the loading on the carbon fines is much higher than on the coarse carbon particles. As the carbon fines are carried downstream and into contact with more dilute solutions, some of the loaded gold will desorb again. While this has not removed any gold from the system, it distributes the gold along the cascade. The gold solution concentration at the top of the cascade is lower than it should be and hence the carbon in the top tank will not adsorb the theoretical amount of gold. Meanwhile, the solution concentration lower down in the cascade is higher than it ought to be, and hence the scavenging effect of the fresh carbon is reduced.

4.2.3 Effect of Frequent Small Transfers

A simulation was carried out (Figure 26) to compare the effect of transferring half the amount of carbon (2500 kg) every eight hours with the base case above (section 4.2.1) where 5000 kg were transferred at 16-hourly intervals. The total amount transferred is still the same, the pumps have to pump for approximately the same total length of time, and therefore the running costs of the two schemes should be roughly equal. It is therefore interesting to see whether the efficiency of the adsorption section could possibly be improved without any extra cost being involved.

Unfortunately the efficiency of this transfer scheme was only slightly higher, at 98,09 %, which may be a result of the timing of the efficiency calculation, as explained above. The gold lockup was slightly down at 47,908 kg, while the amount of carbon was essentially unchanged. While the improvement in efficiency is not exactly overwhelming, the next section investigates the extension of this idea, to see if a trend in this regard can be determined.

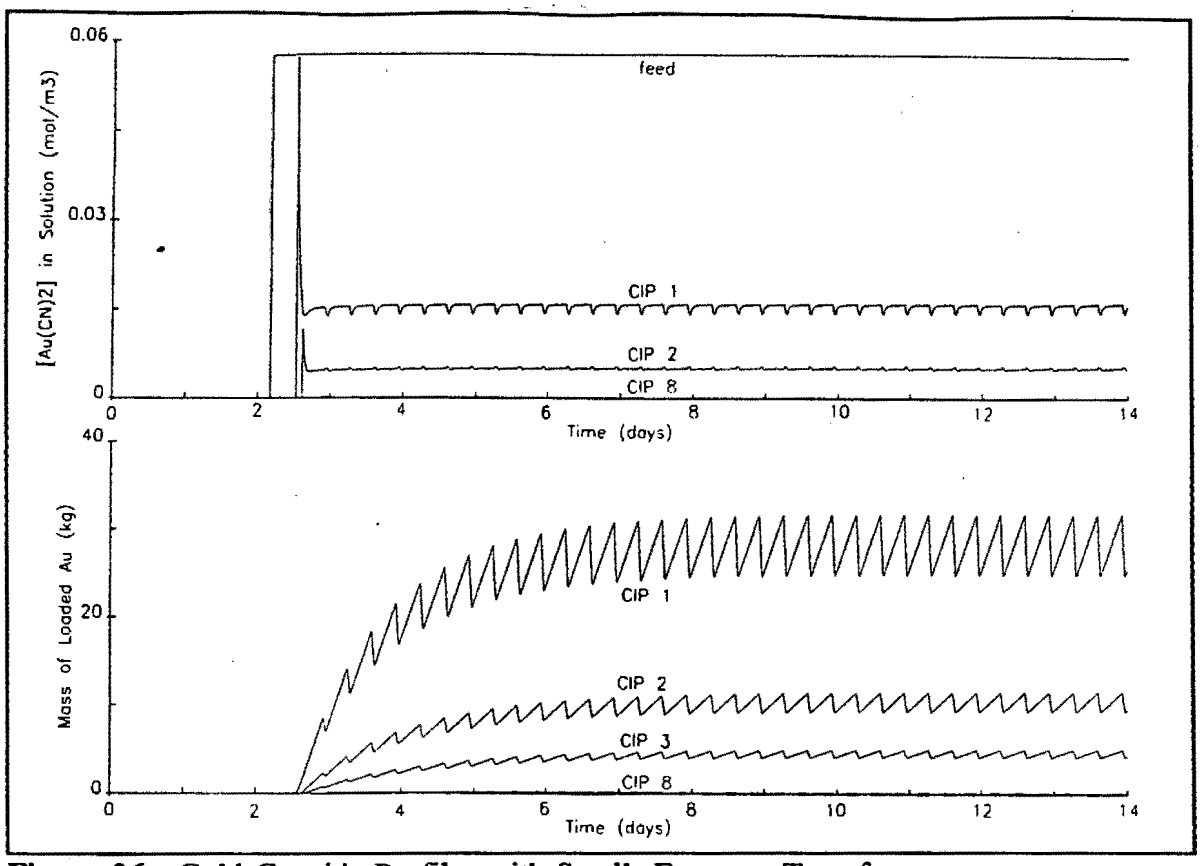


Figure 26 : Gold-Cyanide Profiles with Small, Frequent Transfers

4.2.4 Effect of Continuous Transfers

The continuous method of transfers was one of the usual transfer schemes used in early simulators. It is relatively easy to program, as the transfer streams do not have to be started and stopped at all. Unfortunately this transfer scheme is difficult to implement in reality, as the transfer pumps would have to run continuously, which would simply be impractical on most plants, as maintenance would be difficult or standby pumps would have to be provided. The resulting smooth profiles (see the gold solution and loading profiles in Figure 27 for instance) are certainly more appealing than the saw-tooth results of periodic transfers, though.

If the trend observed before of increased efficiency with an increase in the number of transfers (but keeping the amount transferred the same) was correct, then the continuous transfer scheme should be the most effective with respect to transfer frequency and duration. It is the extension of the investigation into the effect of smaller more frequent

transfers, as it represents the ideal case of an infinite number of infinitely small transfers. If the transfer flowrates are then set so that the same amount of carbon is transferred in a day as in the two previous transfer schemes, the efficiency would be expected to be even higher than the efficiency of the case where small transfers were made every eight hours.

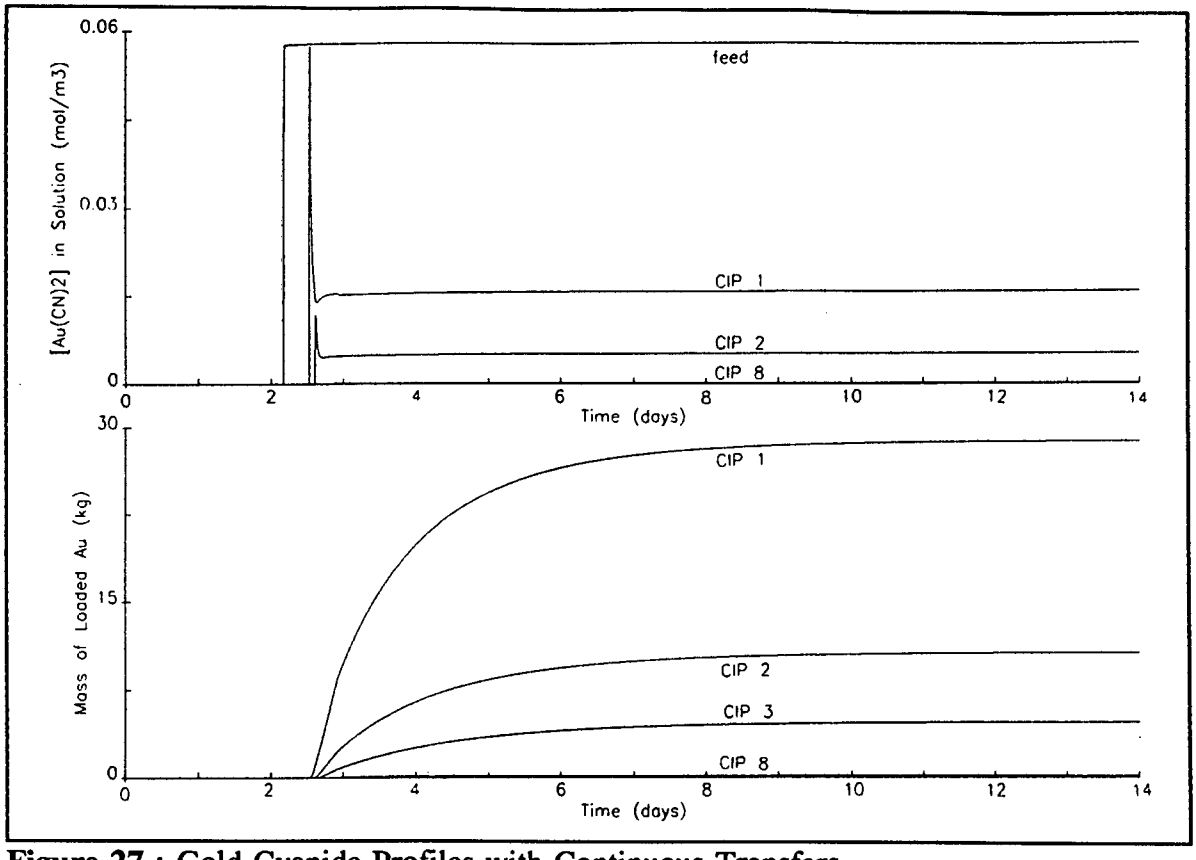


Figure 27 : Gold-Cyanide Profiles with Continuous Transfers

Unfortunately the calculated efficiency was actually slightly lower at 98,08 %, with a slightly higher gold lockup of 48,371 kg. The reduction efficiency may be due to the slightly higher mass of carbon in the tanks (with an average of 5685 kg) which caused the higher gold lockup and hence allowed less gold to be recovered. Essentially, though, the size and period of transfers seem to have hardly any effect on the adsorption efficiency. Instead the total amount of carbon transferred is likely to be of much greater importance: In the continuous transfer method the flowrate of fresh carbon needs to be reduced to such an extent, that the total amount of carbon transferred will be equal to the total transferred with the other transfer schemes. Calculating the correct flowrate is obviously not difficult, but it was found that even very small rounding errors caused considerable errors in the amount transferred over a two week period.

The reduced efficiency (apart from having been caused by the inaccurate method of calculating the efficiency) is thus most likely the consequence of the sensitivity which the process exhibits to the magnitude of the fresh carbon flowrate. To see what effect a smaller transfer flowrate in continuous transfers would have on the efficiency, another simulation was run in which the flowrate was reduced by half. Only half the amount of carbon transferred before was therefore transferred in this case.

As can be expected more gold loaded onto the carbon because the contact time was twice as long as it was before and the total gold holdup increased to a massive 90,318 kg. As the gold loading lay closer to its maximum loading where desorption becomes important, the rate of loading will have been slower than before. This is especially so in the first tank where most loading should occur and where the highest loading is encountered. It is therefore to be expected that the efficiency should be lower by a significant amount, which it is at 97,78 %. The average mass of carbon in all the tanks was closer to the ideal 5600 kg at 5658 kg than for the case with the larger transfers.

4.2.5 Effect of Consecutive Transfers

Another method of transfer entails the consecutive switching on of transfer pumps only when the previous transfer has been completed. The advantage of this transfer scheme, if it is carried out from the top to the bottom of the cascade, is that either the concentration of carbon in the destination tank or the amount of carbon transferred can be controlled easily. To have a better point of comparison with previous simulations the amount of transferred carbon was controlled instead of the concentration in the tank - which would be the usual choice on a plant. The gold cyanide concentration in solution and on carbon are shown in Figure 28.

The efficiency for this transfer scheme is low (97,66 %). The main problem is the size of the transfer: 5000 of 5600 kg available are to be moved out of the tank before any new carbon is added. Especially towards the end of the transfer the concentration of carbon in the pulp is very low, requiring a lot of pulp to be moved to transfer only a small amount of carbon. As a result transfer times are very long, and at least one tank usually

contains nearly no carbon with an associated very low adsorption capacity. It is therefore not surprising that the average mass of carbon in the tanks was only 4294 kg and the holdup of carbon was very low at 31,9 kg.

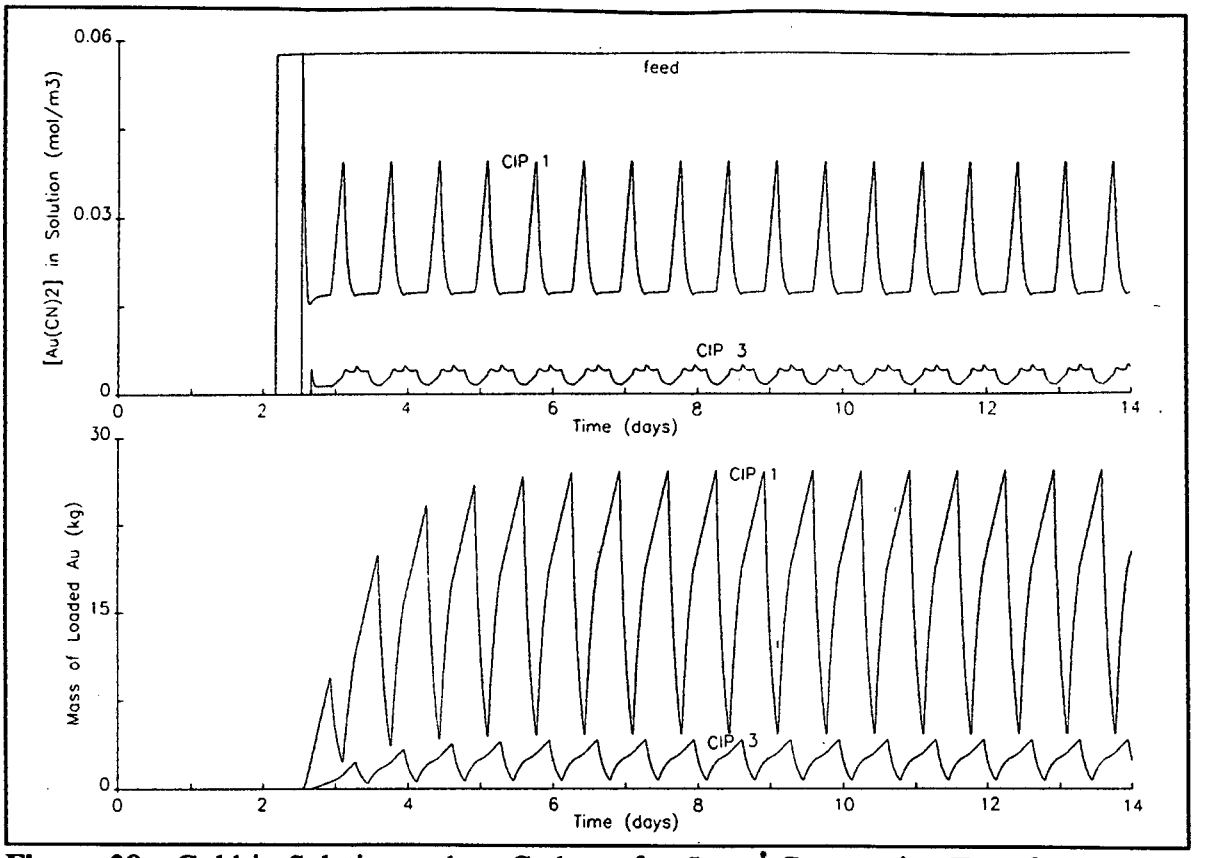


Figure 28 : Gold in Solution and on Carbon after Large Consecutive Transfers

In this case smaller transfers would be expected to be beneficial, as transfer times are much shorter (there would be no problem with too little carbon in the source tank). That is why another simulation run was performed using small transfers (2500 kg) which are started in the top tank every eight hours. The average mass of carbon in the adsorbers is still slightly lower than for simultaneous transfers but, as expected, the efficiency is higher at 98,07 %.

One problem with consecutive transfers which was experienced in both simulations, is that one transfer sequence would be started (this is done at regular intervals) before the previous one could be completed, so that more than one tank would not be at peak performance at any given moment. Also this transfer method would be impractical on a plant with manually controlled transfers as the pumps would have to be started and

stopped at frequent and unpredictable intervals.

4.2.6 Effect of Leaking Carbon

On most plants the screens are far from perfect. From the constant flow of abrasive pulp through the screens, the holes wear out and apart from the normal carbon fines larger pieces of carbon begin to pass through. The shape of a carbon particle often determines whether it will pass through the screens or not, with flat or oblong particles more likely to pass through than round ones of the same volume. To see what effect this has on the efficiency of the plant, a simulation was run in which a leakage function was included, which allows 0,1% of the carbon in a tank to leak out through the screen per second.

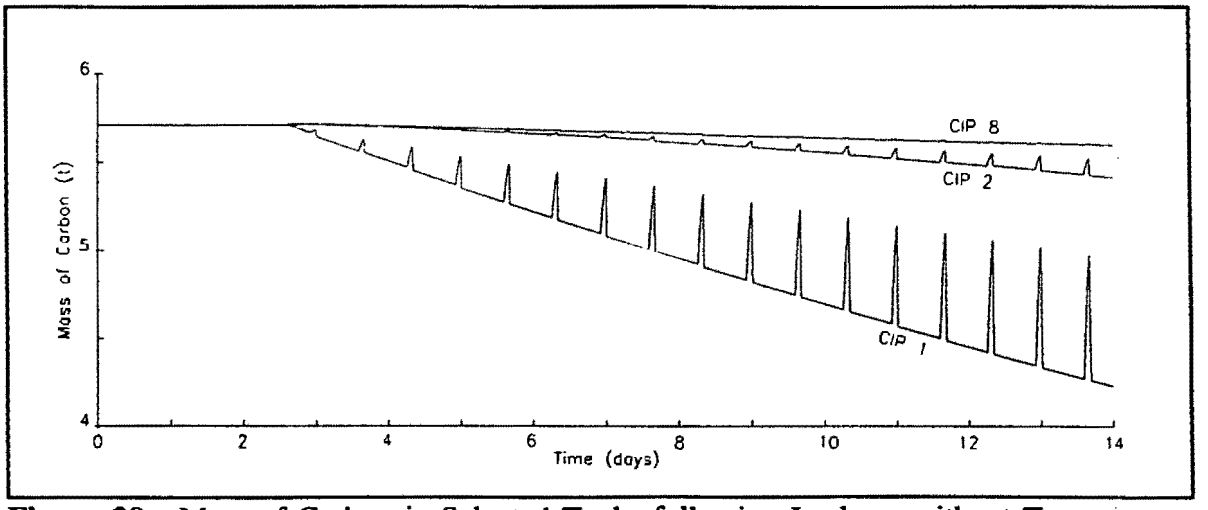


Figure 29 : Mass of Carbon in Selected Tanks following Leakage without Top-ups

Initially the carbon transfers were kept at a constant magnitude, allowing the concentration of carbon to drift over the two week period. What essentially happens (see Figure 29) is that only the concentration of carbon in the first tank drops significantly. The carbon in the feed and outlet streams of all the later tanks is roughly equal, even off-setting the effect of the carbon attrition to some degree. The efficiency is very close to that of the base case (98,01 % as compared to 97,99 %), while it should intuitively have been slightly lower. The total amount of gold locked into the carbon in the cascade is less than before though, as expected. Actually the only tank that contains less gold than before is the first, while all the other tanks actually have more gold locked into the carbon than before.

To study the more realistic case of carbon leakage, where the concentration of carbon in each tank would be controlled rather than the size of the transfer, a scheme was introduced (such as is used in practice on the plant) in which the transfer pumps are restarted individually after normal transfers, to top up the mass of carbon in each tank. The top-up transfer times are relatively short, visible in Figure 30 as the almost vertical lines on the left side of every saw tooth. Top-ups ensure that the mass of carbon in the top tank drifts only over the short period between transfers and is restored to normal levels during transfers.

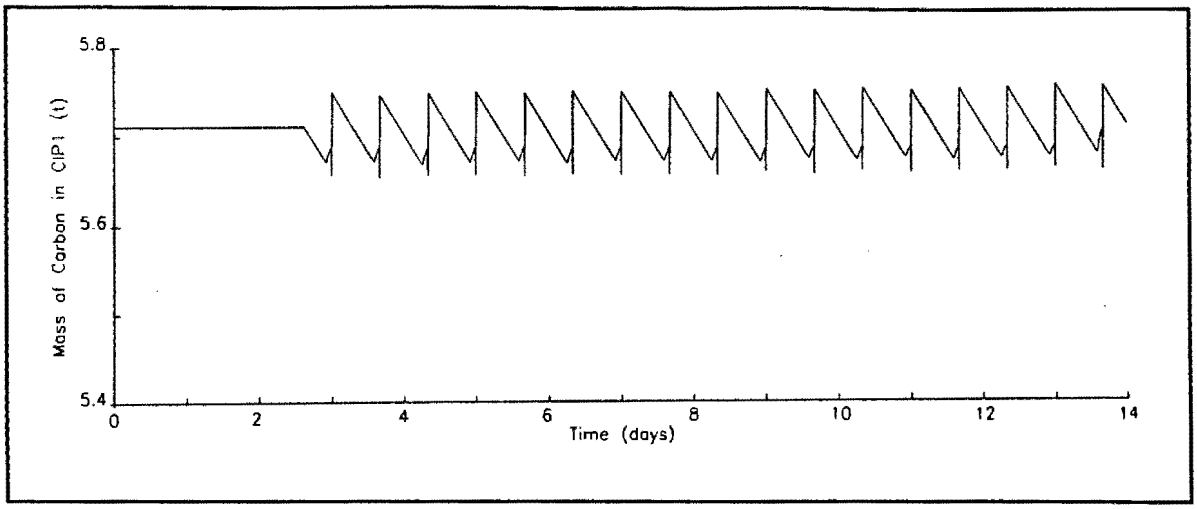


Figure 30 : Mass of Carbon in Selected Tanks following Leakage with Top-ups

The average mass of carbon in this case is higher than before (making up nearly exactly the specified volume concentration of 2 %, or 20 $ml.l^{-1}$). The gold holdup is correspondingly higher and the efficiency is lower, even if only marginally so, at 97,97 %. Essentially it seems that carbon leakage - in contrast to attrition - does not affect the running of an adsorption circuit too badly as long as the concentration of carbon in all tanks is maintained.

4.2.7 Effect of a Non-uniform Carbon Profile

It has previously been reported (Stange et.al., 1990a) that a carbon profile loaded toward the bottom end would be more effective for carbon-in-leach (CIL) applications. It was therefore decided to investigate what the effect would be of loading certain tanks with carbon more heavily than the rest.

Two cases were studied. The first involved adding 1,5 times the normal amount of carbon to the first three tanks of the cascade, while leaving all the others with the usual amounts. With the larger amount of carbon in three of the eight contactors, it is not surprising that the holdup of gold increased, while the efficiency decreased (to 97,73 %).

In the second case, 1,5 times the normal amount of carbon was added to the three tanks at the lower end of the cascade. This effectively increased the scavenging action of the last contactors and increased the efficiency of the adsorption section to 98,11 %. That is the highest efficiency value recorded for all simulations which took attrition into account.

While the increased mass of carbon in the lower contactors was effective in removing more of the gold from the dilute solutions encountered there, the weighting of the carbon profile towards the lower end of the cascades is usually avoided in the plant situation. The reason lies in the increased length of time that the carbon has to spend in the lower contactors, where it absorbs not only gold, but also all sorts of organic and inorganic foulants. As this carbon is pumped upstream its loading capacity for gold has been reduced, counteracting the beneficial effect of the extra amount of carbon. Very often the foulants (especially the inorganic ones) are not removed to a satisfactory degree during the acid wash and regeneration steps, leading to a long-term reduction of efficiency.

This particular simulation seemed more efficient only because the effect of foulants was not included in the present form of the simulator. A smooth carbon profile, in which the carbon can be moved up the cascade as fast as possible, is therefore the usual and correct one to choose in any practical situation where problems with organic or inorganic foulant are to be expected. Only in a relatively clean system would the loading of the bottom end of the cascade be beneficial.

4.2.8 Effect of Regular Transfers with Unequal Flowrates

The flowrates of the transfer streams at the gold plant from which data was acquired, change with time. The highly abrasive pulp wears away the pump impellers so that the flowrates slowly decrease. As fixed speed pump are used, the only way of speeding them

up without replacing the impellers is by an improvised system of using ever larger differential ratios within the driving mechanism of the pump. Usually the exact flowrates are not known and are adjusted according to rules of thumb. They were measured especially for this project with a clamp-on flowmeter and were found to lie in a range of $7{,}1 \cdot 10^{-3}$ $m^3.s^{-1}$ to $2{,}9 \cdot 10^{-2}$ $m^3.s^{-1}$.

To see what the effect of this distribution of transfer flowrates is, a simulation was run in which all transfers were started together at regular intervals of 16 hr, but each transfer then continued for as long as was necessary to move the specified mass of carbon. Intuitively one would expect that this should not have a very pronounced effect on the efficiency. This is mirrored in the results which indicate an efficiency (98,08 %) only just larger than for the base case. This higher efficiency may be caused by the higher mass of carbon in the upper tanks for which the incoming carbon transfer stream has a higher flowrate than the exit transfer stream, so that for a short time the mass of carbon in these tanks is higher than usual. This assumption is supported by the slightly higher average mass of carbon in the tanks than during normal operation (5711 kg as compared to 5600 kg).

4.2.9 Effect of Irregular Transfers and Equal Flowrates

The efficiency of the adsorption process with irregular, nearly random, transfers is far worse than the efficiency achieved with the regular transfers encountered until now. On the plant simulated in this project it was observed that the carbon transfers are poorly coordinated: The pumps are seldomly started at the same time or in a specific sequence. Some pumps are then left running for long periods, while others are stopped almost immediately.

As an example the on/off signals of the transfer pumps that transfer carbon into and out of CIP contactor 4 are shown in Figure 31, as they were recorded on the plant, together with the resultant mass of carbon in the contactor. As the two pumps were not coordinated, the tank sometimes contained more than double the amount of carbon which it is designed to hold (see day 9) and then for about 3 days at the end of the week it

contained just about no carbon at all. This is not an unusually bad example, but rather shows what effect the unsatisfactory control of carbon transfers has.

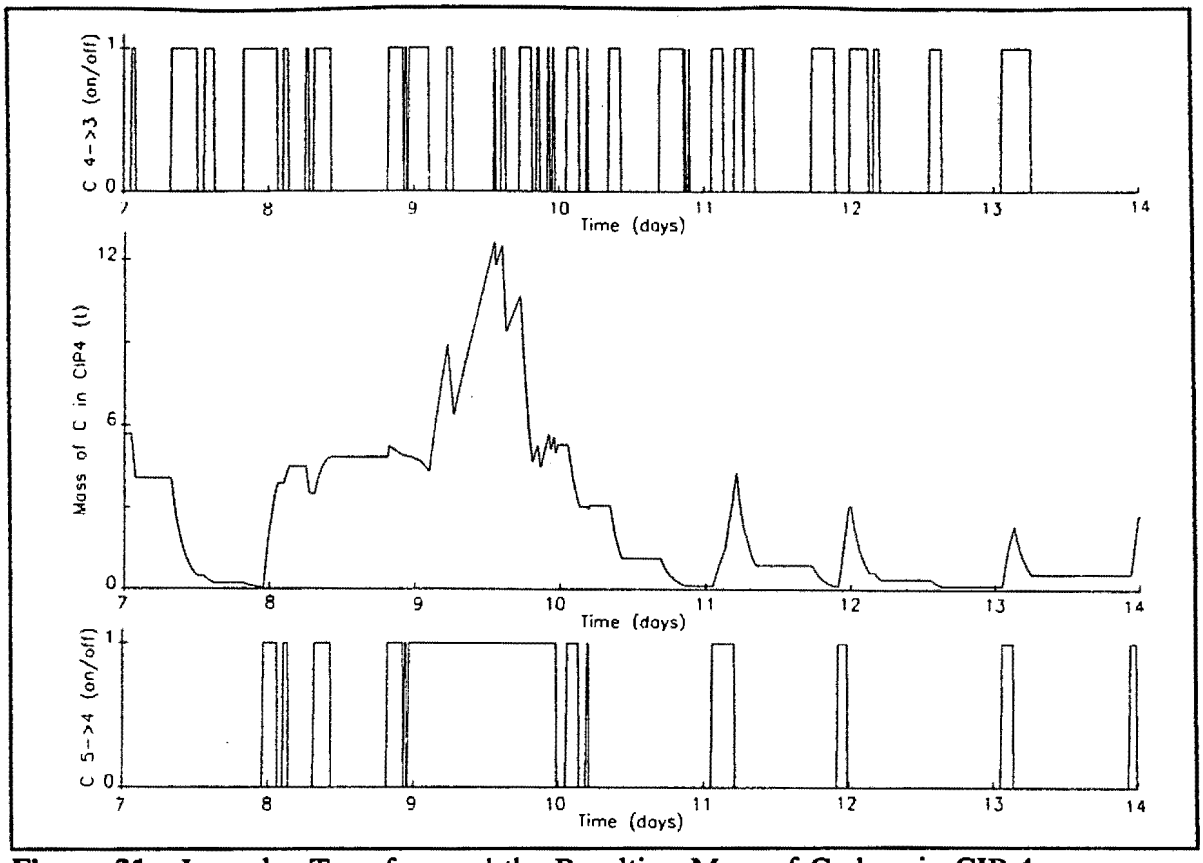


Figure 31 : Irregular Transfers and the Resulting Mass of Carbon in CIP 4

Part of the fault must lie with the inaccurate method in which the carbon concentration is measured: a sample of pulp is taken from the tank and is poured through a small screen. The carbon retained in the screen is rinsed under running water and is then washed into a little measuring cylinder where an approximate measure of the volume of carbon is taken.

If the carbon concentration is too low, as determined by the illustrated method, the transfer to the tank should ideally be restarted to rectify the concentration. Similarly, if the concentration is too high, more carbon should be transferred from the tank in question to the one above. But again no information exists on how long these equalization transfers should be kept going and essentially the performance of the plant depends on the feel which the operator has developed for corrective action. With such an - at best - subjective method of control, a plant will usually not operate at design carbon concentrations.

This situation was simulated by using the irregular periods of transfers as recorded on the plant. These transfers periods were read into the simulator (with equal transfer flowrates) and caused the efficiency of the adsorption circuit to drop to 96,62 %. This is hardly surprising if one considers how the concentration of carbon in the contactors varies with time.

4.2.10 Effect of Irregular Pulp Flowrates

As has been discussed earlier in section 4.1.4, the pulp feed flowrate to the leach section fluctuates greatly. The interconnectedness of the leach pachucas smooths out the worst of the fluctuations, but cannot prevent the feed to the CIP from also fluctuating and this particular simulation was run to see what the effect of these fluctuations would be. The carbon transfers were the same equally sized transfers simultaneously started at 16 hr intervals as in the base case.

The results indicated that the effect of the fluctuations is not as bad as it was in the leach. The efficiency has still dropped to 97,75 %, though, with the average carbon mass in the tanks at normal levels, but the gold holdup slightly higher at 54,4 kg. The higher holdup is a result of the greater loading on the available carbon caused by the increase in the gold cyanide concentration coming from the leach.

4.2.11 Effect of Irregular Unequal Transfers and Irregular Pulp Flowrate

The effect of having both an irregular feed and also transferring carbon at irregular intervals, for varying lengths of time and with different flowrates as happens on the plant is expected to be especially inefficient. This expectation is confirmed by the simulation efficiency for this run, which lies at 96,15 %. The cumulative effect of these factors resembles normal plant conditions most closely. Figure 32 shows both the solution concentration profiles of $Au(CN)_2^-$ and the gold loadings on carbon.

The fluctuations of gold on carbon in the first tank are quite remarkable. Note how nearly all the additional gold being carried into the first tank by the more concentrated feed

solution is adsorbed by the carbon in this tank. The mass of gold on carbon in the first tank rises as the feed solution concentration rises, while the gold solution concentration in the first tank changes only slightly. The mass of adsorbed gold in the second and all following tanks similarly increase only to a very small degree.

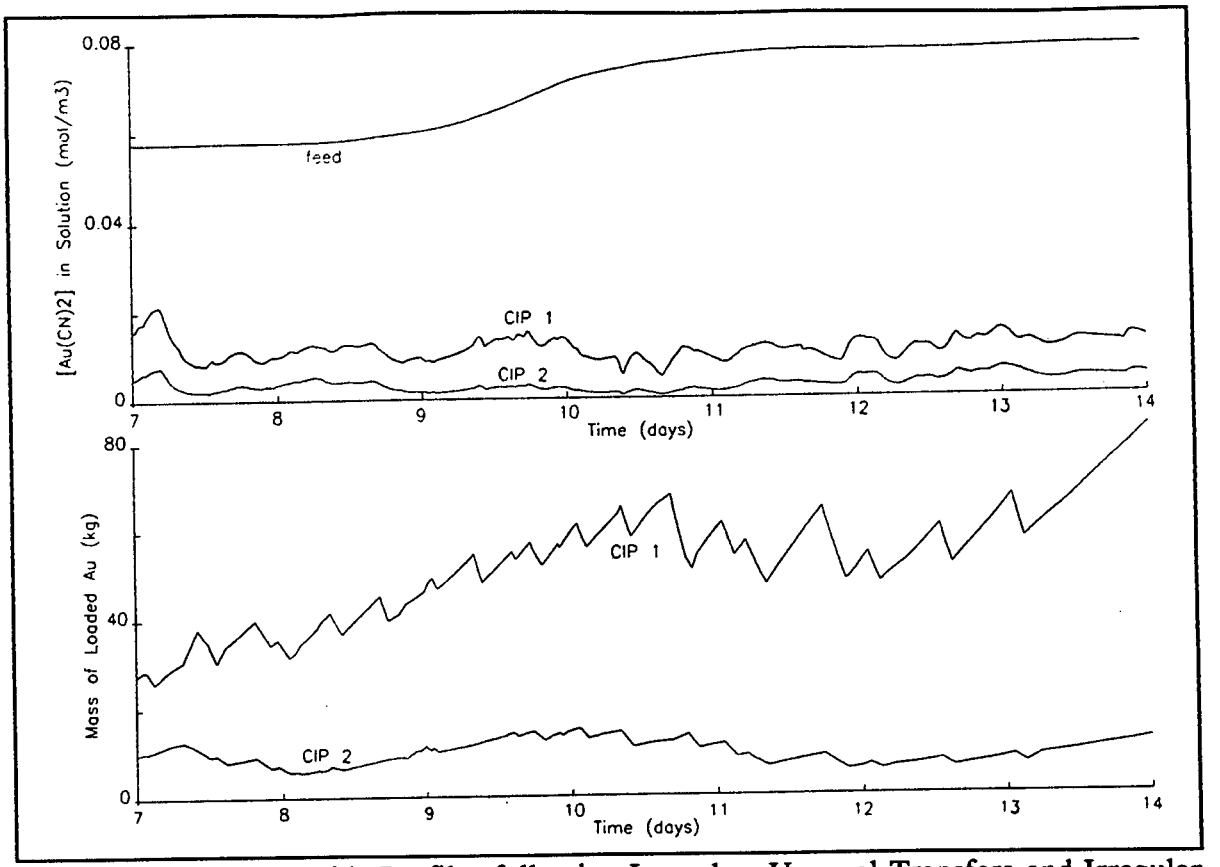


Figure 32 : Gold-Cyanide Profiles following Irregular, Unequal Transfers and Irregular Feed

4.2.12 Effect of a Screen Overflow

In the ideal plant as symbolised by the base case, the effect of an overflow on the CIP efficiency is insignificant (the efficiency was the same as for the base case at 97,99 %). The duration of an overflow as simulated is about 20 min, but the amount of carbon carried downstream is not very large (only about 400 kg, or 7 % of the carbon in the tank) resulting in the slight imbalance of carbon in tanks 1 and 2 as shown in Figure 33. In reality the amount of carbon carried downstream is likely to be larger, but because of the limitations of the simulator with respect to the sequence and timing of events, the above approximation had to suffice.

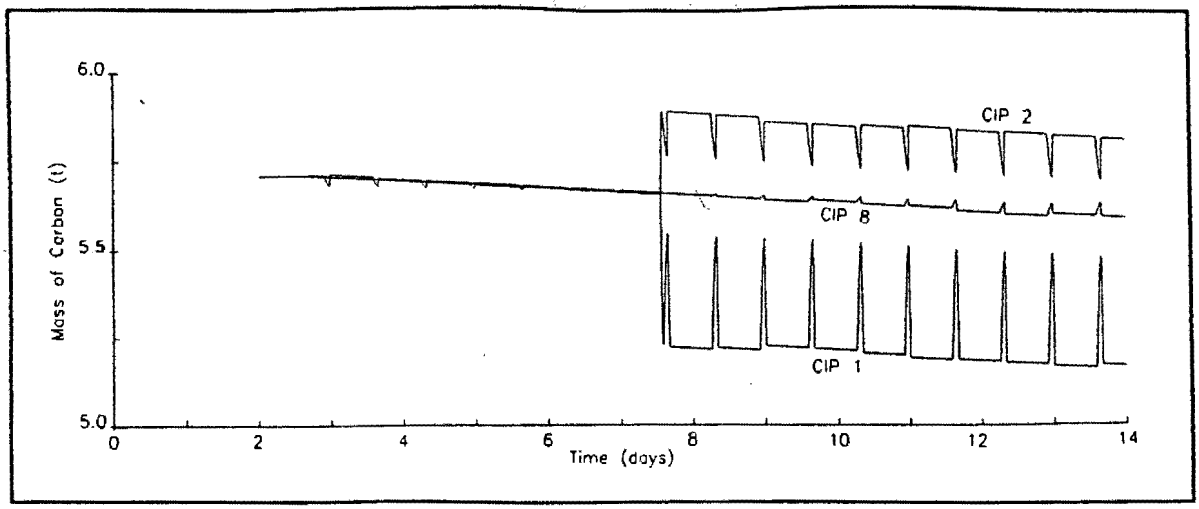


Figure 33 : Mass of Carbon in Selected Tanks following an Overflow in CIP 1

The simulator has to run through the sequence of events as outlined in section 3.3.2.4 for a single tank by assuming that this is possible without a hitch and without affecting other tanks. In reality a single blockage can cause a whole chain reaction of further blockages as the result of attempts to unblock the previously blocked tanks. To rectify the operation of the adsorption section, it may become necessary to shut off the feed to the CIP cascade completely and to separately unblock each one of the screens. Such an operation may put the whole CIP train out of action for an hour or more.

A second reason for the small quantity of carbon to be carried downstream lies in the limits set in the simulator. Carbon is assumed to be carried downstream only during the time spans between overflowing into the screen and the closing of the exit valve, and from unblocking until the pressures within and outside the screen have normalised. All the carbon which was carried over into the screen before normal operation is again restored will in reality be washed downstream afterwards, but this is ignored by the simulator. The reason for this limitation lies in a conscious decision to keep the number of variables small: had the overflow of carbon been modelled realistically, an extra state variable would have been needed for each tank to keep track of the carbon which is located above the screen.

On the other hand the simulation also takes a worst case approach by assuming that the concentration of carbon in the tank which overflowed will not be restored at the next

transfer, but that only the usual amount of carbon will be moved. (Figure 33 shows that the mass of carbon in tank 1 remains below design levels after the overflow.) This creates a distributed carbon profile with less carbon in the first tank and more in the second. The short term effects of allowing the more highly loaded carbon to move downstream are outweighed by the long term effects of the new carbon distribution. During the actual overflow it was reported above that approximately 7 % of the carbon from tank 1 is lost to tank 2. This means that 7 % (or 1,9 kg) of the adsorbed gold in this tank must also have leaked downstream. Meanwhile, at the end of the week the total amount of gold recovered was only 0,55 kg less than that recovered in the base case. This implies that the reduced mass of gold adsorbed by the smaller amount of carbon in the first tank caused the solution concentration in this tank to rise. The higher solution concentration in turn forced more gold onto each particle of available carbon. Hence having less carbon, which is more highly loaded, reduces the overall recovery only slightly.

In the case of the non-ideal plant as outlined in section 4.2.11 an overflow in the first tank further reduced the efficiency from 96,15 % to 96,13 %. This means that the overflow reduced the amount of gold retrieved by 56 g. This loss is hardly significant, but the exact time of overflow was possibly not well chosen, as the concentrations of carbon in both tanks were very high and the effect of the overflow was negligible.

Overflows do reduce the overall efficiency of the CIP circuit and cause gold to be lost. However small the amounts lost seem to be, it would still be wise to avoid them if possible.

4.3 GENERAL DISCUSSION

For the Measurement and Control Division at Mintek the question which naturally arises is what the results presented above imply for the past and future development of measuring instruments within the Division and the possible control applications in gold plants. In an extensive drive over the past decade the Division has come up with a number of novel instruments and in these economically hard pressed times one would like to know whether any further development is justified. Should one market the available instruments more aggressively using the new information or does it reveal that these instruments and control applications are unlikely to produce the expected improvements ?

The plant management at the same time would like to know how the profitability of the plant can be increased by spending as little extra money as possible. The poor performance of gold over the last year has reduced the amount of money available for fancy and expensive controllers. Yet at the same time the shareholders still want the maximum return possible on their investments and efficient control is one of the best routes of ensuring maximum profitability.

A final answer is obviously beyond the scope of this dissertation, but the new insight that was gained can be used to partially answer the above questions. The factors which have been investigated all apply to the particular case of the gold plant modelled. The variables which were monitored by the plant computer over the months of the Mintek data-logging project were combined as far as possible with the extra information gained through measurements of physical plant parameters and the analysis of samples taken on the plant. Any insight gained will therefore apply directly only to the plant in question, but it is possible to apply them to other similar operations if the limitations of the analogy are kept in mind.

Many of the factors which were investigated are interdependent so that it is sometimes difficult to see exactly what the effect of each separate one is. At the same time the interdependencies themselves are important and will be highlighted where necessary.

4.3.1 Fluctuations in the Feed Flowrate

The one factor which is most noticeable when looking at the performance of the plant on the plant computer is the flowrate of feed pulp to the leach. The fluctuations in the flowrate are enormous and always present. Upstream processes and the set points chosen by the operators contribute to the constant change in the volume of pulp flowing to the leach.

The upstream processes which have an influence are i) the mine, with varying amounts of ore supplied, ii) the mills, which react differently to varying rock hardness etc., and iii) the thickeners. The thickeners are built to provide a pulp with an essentially constant density to the leach. They have an enormous capacity for pulp but can only be used to a very limited extent as buffers between the mills and the leach. The pulp flowrate coming from the thickeners is controlled by a cascade controller which ensures that the density remains constant. For the leach a constant density is convenient because it makes the cyanide addition easier to control: It was explained earlier already that the higher the density of the pulp is, the more gold will be available to be dissolved. This means that more cyanide will have to be added to dissolve all the gold. At the same time, the smaller water fraction will have to carry more aurocyanide in solution, implying that the solution will need to become more concentrated. For cyanide addition control it is therefore best if the density remains roughly constant.

When the density in the thickener underflow is too low, the flowrate is reduced to give the particles in the thickener more time to settle which produces a pulp with less water. If, on the other hand, the density is too high, the flowrate is increased to reduce the time available for settling. The density control is very tight giving it a fast response and it is therefore often misused:
The only way of cutting the flow of pulp from the thickeners, while leaving the cascade controller on automatic is to increase the density set point. This is the control action chosen when, for instance, the leach pachucas are too full because the flow to the CIP had to be stopped or because spent eluate is being added. It was also the remedy chosen when a problem with the supply of process water was being experienced: the density set point

was increased so that the pulp being delivered to the leach was as dense as possible and more water was available to be returned to the mills. These adjustments to the density set point are unfortunately all too frequent.

Overall the density and flowrate of pulp flowing to the leach fluctuate significantly, contrary to the original design specification. To calm the system down it would be beneficial to use the buffering capacity of the thickeners to the maximum extent without unduly interfering with the operation of the thickeners. Normal operation of the plant implies that the effect of density is not critical enough to warrant the tight control which it is receiving. Even though density was not considered separately in this dissertation it would seem that the system can handle changes in density satisfactorily as long as the cyanide addition is adjusted. The fluctuations in flowrate are detrimental both to the leach efficiency as well as the adsorption efficiency (the efficiency of gold retrieval was reduced from 97,590 % for the base case to 97,314 % for the case with plant recorded flowrates). The plant is therefore likely to become more efficient if the fluctuations in flow of the feed to the leach were reduced. This could easily be done (without installing any additional controllers) by relaxing the tight control on the density somewhat and thereby reducing the exaggeratedly fast flow adjustments required for this tight control.

This change in control strategy was already suggested during the data-logging project but practical problems prevented its implementation. The operators have become accustomed to controlling the level in the leach with the density set point on the thickeners. A change in the control scheme would remove the most effective method available to the operators for handling upsets in the leach or the CIP. The operators would therefore have to be retrained before such a change could be implemented.

One major disturbance in the leach, for which a suitable control mechanism to cut back on the amount of feed pulp is required, is the addition of spent eluate. A fairly large volume of solution is usually pumped from the smelt house to the top of the leach in a short time span. Accordingly, the levels in the leach rise suddenly and very often the feed to the leach has to be trimmed. Initially the extra volume of pulp is absorbed by the pre-leach aeration tank but as this has only a relatively small buffering capacity, the thickener

underflow stream has to be reduced as well.

The best solution to the problem (which was already suggested during the data-logging project on the gold plant) would be to install a buffer tank for the returned eluate, allowing it to be bled into the process continuously instead of being added in sudden bursts. Apart from reducing the disturbance which the spent eluate presents to the hydrodynamics, this would also have the beneficial effect of making cyanide addition easier, as it would not have to be cut every time spent eluate was added. The buffer tank would obviously require extra capital and if this were not available, the option of adding the spent eluate to the process water storage tank instead of the leach could be investigated. The questions which would have to be addressed are: whether the process water is alkaline enough to prevent the hydrolysis of free cyanide, and what the effect of leaching in the mills and in the thickeners would be.

Similarly the addition of storm water caught in the leach and CIP sumps would have to be diverted from the leach, possibly also to the process water tank. With the feed fluctuations to the leach reduced, the feed fluctuations passed on to the CIP would also be substantially reduced. This is likely to reduce the frequency of screen blockages, which are most likely caused by the increased pressure of pulp on the screens during periods of high flowrates.

4.3.2 Cyanide Control

The addition of cyanide is critical for the efficient operation of the leach. One of the simulations which took the pulp feed fluctuations, the cyanide addition rate and spent eluate additions into account, showed that the efficiency of the leach was 0,182 % less than for the case where cyanide addition was kept constant, resulting in an increase of the discard grade of 20,5 $mg.t^{-1}$.

The amount of cyanide that needs to be added to the leach is much larger than what is needed to satisfy the stoichiometry of the gold leaching reaction. Large quantities of cyanide are consumed by the side reactions, eg. other metals dissolve to form cyanide

complexes and oxygen reacts with the cyanide to produce cyanate. Enough cyanide must therefore always be present to dissolve all the remaining gold despite the destruction in these side reactions. At the same time cyanide is added in excess to drive the reaction forwards.

The fluctuations in the pulp feed flowrate and density and the addition of spent eluate make the control of cyanide concentration in the leach more difficult. The cyanide addition setpoint is chosen by the operator based on information provided by titrations done on filtrate of pulp in the first leach tank. Samples of pulp are taken at regular intervals, are filtered and titrated. As long as the worker has basic training in titrating and especially endpoint detection, this should essentially not be a problem. Unfortunately from discussions held with these workers, it seemed that they did not necessarily understand what they were doing. They would also consciously adjust the readings taken to satisfy the operator without appreciating the consequences. The results that the operator bases his decisions on are thus not the true values and similarly his reaction will be a biased one.

Cyanide measuring instruments are notoriously expensive and must be maintained well to give meaningful results. They all require the pulp to be filtered. The most simple type of analyzer handles only the clear filtrate. More advanced analyzers allow the operator to simply place the pulp sample in the reception vessel, where it will be automatically filtered before being analyzed. On-line instruments have been developed, which employ hydrostatic filters which can be left in the pulp for considerable lengths of time. The instruments are supplied with a constant supply of clear filtrate which is analyzed at intervals of a few minutes. An instrument is being developed by the Measurement and Control Division, which will be able to supply a continuous reading of the concentration of cyanide in the pulp at a significantly lower cost and without requiring the pulp to be filtered.

If a reliable instrument were available to give either a continuous reading or a sufficiently regular non-continuous reading, an automatic cyanide control strategy could easily be implemented. The best option would be to use ratio-control to add the cyanide in proportion to the pulp flowrate. This would make the cyanide controller independent of

attempts to reduce fluctuations of feed flowrate as was discussed above. A slightly more intelligent controller would also be able to take the density variations into account and would be able to adjust the cyanide rate during periods of spent eluate addition - if periodic additions are maintained. The reading of cyanide concentration would best be used in a cascade controller which adjusts the ratio of the cyanide addition rate to the pulp feed flowrate.

The improved cyanide control, if implemented separately from any smoothing of flowrate or spent eluate addition has the potential of increasing the amount of gold dissolved which becomes available for adsorption by over 500 g a week. Depending on which cyanide analyzer is used, the new control strategy would be expected to pay for itself within a time span lying between two to eight months.

4.3.3 Carbon Transfers and Carbon Concentration

The state of carbon transfers at the particular gold plant used in this study is unacceptable if the data logged on the plant is anything to go by. The timing of transfers is not controlled intelligently, transfer pumps are sometimes left running for hours and others are sometimes not switched on for four shifts in a row. With such irregular transfers the carbon concentration in the various tanks cannot be maintained at the required levels.

The simplest strategy would be to let the plant computer start the transfer pumps simultaneously at regular intervals and to stop them after a specified length of time. This would ensure a minimum in regularity and would maintain a relatively constant but possibly distorted carbon profile. The operator should only be able to override the computer in case of screen blockages or some other emergency.

As was discussed earlier in section 4.2.8, the transfer flowrates are not equal and change with time. If all transfers were kept going for an equal length of time, the carbon profile would quickly become distorted. The duration of transfers would therefore have to be adjusted somehow to ensure that the carbon concentrations in all tanks are kept at the correct levels. This could either be done by measuring the transfer flowrates at regular

intervals (eg. once a week) and adjusting the lengths of the transfers as set on the plant computer accordingly. Another option would be to keep the transfer durations for all tanks the same and then to top up the concentration in each tank separately.

Controlling the top-ups is not expected to be easy. It is nearly impossible to get an accurate measure of the carbon concentration in the tanks. The method used on the plant as described previously is inaccurate and should ideally be repeated to give a more reliable value. A carbon concentration meter has been developed to give a continuous reading of the concentration, which also takes the movement of carbon within the carbon into account. If such an instrument were available in each tank, the top-up transfers could be started individually and continued until the concentration in the tank being topped up had reached the correct value. If carbon concentration meters are not available, it would be up to the person starting and stopping the pumps to use his knowledge of the process to estimate the approximate lengths of time necessary for each top-up and possibly doing a check of the concentrations when the estimated time is nearly over. This would be a very laborious process though, and would in all likelihood give no better results than the present system of transfers.

Top-ups will be necessary not only to correct the carbon profile distorted by unequal transfers but also to counteract the effect of attrition and carbon leakage. The leakage of carbon can be picked up by using leakage detectors and can then be prevented (or at least be reduced) by replacing those horizontal screens which have worn out. The plant already has a maintenance schedule, in which the screens are periodically replaced, so this would not present too much extra work. A program such as this may not prevent leakages totally but at least reduces it to acceptable levels. As long as the leaked carbon is compensated for, the efficiency of the CIP should not be affected too badly.

Carbon attrition is a more intricate problem in that it occurs whenever activated carbon is used and it cannot be prevented. As was shown in section 4.2.2, attrition reduces the efficiency of the adsorption section quite significantly. This is not only done by carrying gold out of the adsorption section, but also happens because of the levelling out of the solution concentration profile along the cascade. The only method of reducing the effect

of attrition is to ensure correct hardness of the carbon to start off with and to wash the carbon thoroughly before adding it to the last adsorption contactor.

The efficiency of the CIP depends on the correct maintenance of the carbon profile in the cascade. Even if the implementation of a control scheme would not be cheap or easy, it should definitely be considered if the efficiency of the CIP section is to be improved.

CHAPTER 5

CONCLUSION

The aim of this project was to write a flexible dynamic simulator of the gold leaching and adsorption processes to be used at a later stage for fault finding, optimization and control of existing gold plants. While it was applied to only one specific plant, it was to be flexible enough for quick application to any such operation.

The simulator is written on a molar basis, with mole balances serving as the dynamic equations for the molar species in the reaction units, ie. for the state variables. The pertinent reactions of the major constituents are included, as well as the hydrodynamics of the process units, which allow the transfer of material between reactors to be modelled realistically. Realistic modelling of the hydrodynamics was especially important in the case of the carbon-in-pulp (CIP) section in which complex interactions exist between the adsorption contactors.

The computer program for the simulation was written in Fortran and consists of four main sections:

- The first is the main program, which sets up the variable vectors according to the flowsheet information which it reads in from a data file. The flowsheet information includes the type and number of units and the streams running between them. The flexibility of the program lies in this setting up of the physical process outside the simulator, with the simulator being able to cope with any set of internally consistent data. The main program section also interfaces with the user and stores the results.
- The integrator is based on the Bulirsch-Stoer numerical integration technique. It is an explicit method, which is unusually stable and therefore allows the integration to proceed with very large steps in comparison to other explicit methods. The error in integration is monitored and forms the basis for step-size selection. A special feature was included for

the tracking down and crossing of discontinuities.

- The algebraic variables section calculates the values of all algebraic variables based on the value of the state variables at the same instant. The algebraic variables are all those variables such as mols in streams, mol totals etc. for which no derivatives are calculated.
- The derivatives routine evaluates the vector of derivatives of all state variables using the algebraic variables. The state variables are all the molar amounts of reactants in the process units.

The simulator which has been developed has made possible the investigation of a few of the factors that affect either the leach section, the adsorption section or both. The numerical results allow comparisons relative to base cases to show how strong the effect of each factor is on the efficiency of the respective section. With information gathered on a particular South African gold plant a case study was available with which the relative importance of the effects could be established.

The factors which affect the leach most strongly are the addition of cyanide and the concentration of dissolved oxygen in the pulp, where the latter is not a problem at the plant studied. The amount of costly fresh cyanide needed can be reduced if the addition of spent eluate is properly coordinated. The effect of fluctuations in the pulp feed flow and density does not critically affect the efficiency of the leach. Better control for the thickener underflow should be considered, though, as this represents an inexpensive and easy method of improving the efficiency of the leach. This would also make the addition of cyanide easier to control, which is a much more pressing problem. The efficiency of the leach is usually fairly high but improvements, even if they seem relatively small percentage wise, may translate into large financial returns.

Similarly, the inherent efficiency of the adsorption circuit is high as a result of the special affinity of the carbon for the aurocyanide complex and the counter-current method of contacting the activated carbon and the pulp phase. Various cases have been simulated to show what the effect is of process upsets or the different options which are available in running the process.

Attrition of the carbon is a process which cannot be prevented. It reduces the efficiency significantly, not only by reducing the amount of carbon in the cascade or by carrying gold out to dump but more significantly by upsetting the solution profile in the cascade.

The most effective carbon profile seems to be the one in which the lower contactors have more carbon than the others so that the discard stream is effectively scavenged before being dumped. If problems with foulants are expected, though, the same amount of carbon should be maintained in each tank. The amount of carbon transferred in every cycle should be of the same magnitude as the total amount of carbon contained in the tank. The type of transfer is relatively unimportant, with the simultaneous transfer scheme being the easiest to implement.

Most other factors have an indirect influence on the efficiency by altering the carbon profile in the cascade. For instance, carbon leakages and overflows distort the profile by carrying carbon down the cascade. Similarly badly coordinated and irregular transfers can distort the profile significantly. Meanwhile the choice of the correct transfer scheme is potentially the best tool to stabilize the carbon profile and thereby to compensate for the effect of other disturbances.

The simulator should possibly be extended by including the effect that process conditions have on the various reactions (eg. pH and temperature). Another effect which seems important and should be investigated is the competitive loading of the various species on carbon.

Overall this study has highlighted the possibilities of improving the efficiencies of the gold recovery processes, partly through simple control of feed flowrates and addition of major reagents. A more sophisticated control system may have to be developed to maintain the optimal carbon profile and ensure maximum adsorption efficiency in the CIP section.

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APPENDIX I : PRINT OUT OF THE COMPUTER PROGRAM

I.1 SIMU.F : MAIN PROGRAM

```
C ***************************************************************************
C                                                                            *
C       Program to simulate the gold-leaching and adsorption process         *
C       ____________________________________________________________         *
C                                                                            *
C       This is a simulation of a leach cascade of a variable number         *
C       of CSTR's and a CIP cascade, also with a variable number of          *
C       adsorption vessels.The simulation can start with empty tanks         *
C       to simulate the start-up of the plant. Another option is to          *
C       carry on from where the last simulation ended or as a third          *
C       option, steady state data for a fixed number of filled tanks         *
C       can be read in from a data file. Dynamic plant data is read          *
C       in from plant data files.                                            *
C                                                                            *
C       The variables are divided into state and algebraic variables         *
C       which are contained in separate condensed vectors (X and A).         *
C       The individual variables (mols, volumes or mols/s) are refe-         *
C       renced by means of the starting position indeces (INX and            *
C       INA) for each unit, stream or connection.                            *
C                                                                            *
C       The plant configuration data is read in from PLNT.PDT (ie.           *
C       number and types of units, number and direction of streams           *
C       and connections). The stoichiometric constants (STOI) and            *
C       reaction rate constants are read in from CHEM.DAT. The phy-          *
C       sical constants of each species (PHYS[1] = molecular mass            *
C       (in kg/kmol), PHYS[2] = relative density (in kg/l)) are read         *
C       in from PHYS.DAT and are used to calculate the molar volumes         *
C       CONV (in kmol/m3)                                                    *
C                                                                            *
C       Information on the species, reactions and plant set-up used          *
C       in the present configuration is available in the file PLANT.         *
C       DOC.                                                                 *
C                                                                            *
C       The integration is performed using the Bulirsch-Stoer method         *
C       which is called via the ODEINT subroutine in file BSINT.FOR.         *
C       The derivatives needed by the integration routine are called         *
C       in the DERIVS routine (in file DERIVS.FOR), which in turn            *
C       calls the routines in ALGUS.FOR to calculate all algebraic           *
C       variables.                                                           *
C                                                                            *
C ***************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2,  NREAC = 12)
      PARAMETER (KMAX  = 10)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                 + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,TT,ZERO,CONV,VOL,PI,TRLIMIT,GOLD,
     &  AUCN,CCLIMIT
      DOUBLE PRECISION VTNK,VSCR
      DOUBLE PRECISION XP,AP,T1,T2,TE,DT,TSAV,tsav2,TP,H1,HMIN
      INTEGER UNIT, STREAM, CONN
      CHARACTER ANS
```

```
      PARAMETER (ZERO = 0.0, PI=3.141592654, TINY=1.0E-30)
      DIMENSION X(NSTAT),A(NALGB),FLO1(NSTRM),HLA(NUNIT),
     & HLD(NUNIT)
      EXTERNAL DERIVS,BSSTEP

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),CONN(NCONN,2),
     &               INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /DIRIV/ STOI(NTYP2,NCOMP,NREAC),RK(NTYP2,NREAC)
      COMMON /MNNDV/ KALLS,KALLS2,KROUND
      COMMON /FEEDS/ OPTSIM,DAT(18),LUAT
      COMMON /OPTNS/ OPT2,OPT3,TRLIMIT,OPT4,CCLIMIT,NCOND2,
     &               OPT5,OPT6,OPT7,OPT8,OPT9
      COMMON /UNICO/ MUNIT(NTYP1),LUNIT
      COMMON /CARBN/ FLO(NSTRM),IBLK(NUNIT)
      COMMON /PATH/ XP(NSTAT,KMAX),AP(NALGB,KMAX),TP(KMAX),
     & TSAV,DTSAV,KOUNT

C     READ FORMATS:
5     FORMAT (1X,F4.1,1X,F4.1,1X,F4.1,1X,F6.3,1X,F6.3,1X,F6.3,1X,F6.3,
     &        1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,
     &        1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1)
15    FORMAT (1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,
     &        1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,
     &        1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1,1X,F4.1)
25    FORMAT (1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4,
     &        1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4,1X,E9.4)
35    FORMAT (1X,E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X
     &        E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,
     &        E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,E11.5,1X,
     &        E11.5,1X,E11.5)
45    FORMAT (F11.2,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &        E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &        E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &        E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,F11.2)
55    FORMAT (3X,I6,2X,F6.2,2X,F6.2,2X,F6.2,2X,F6.3,2X,F6.3,2X,F6.2,
     &        2X,F6.2,2X,F6.2,2X,F6.4)
65    FORMAT (I6,3X,F7.7,3X,F7.7,3X,F7.7,3X,F7.7,3X,F7.7,2X,F3.3,
     &        2X,F3.3,2X,F3.3,2X,F3.3)
75    FORMAT (I6,2X,F3.1,2X,F3.1,2X,F3.1,2X,F3.1,2X,F3.1,2X,F3.1,2X,F3.1,
     &       2X,F3.1,2X,F3.1,2X,F3.1)
C     WRITE FORMATS:
115   FORMAT (I6,3X,F9.4,3X,F9.4,3X,F9.4,3X,F6.4,3X,F6.4,3X,I4,I4)

C     START CALCULATION
C                                                          read in plant configuration data
      DO 10 M=1,NTYP1
        MUNIT(M) = ZERO
10    CONTINUE
      OPEN (14, FILE='plnt.pdt')
      DO 30 I=1,NUNIT
        READ (14,'(1X,I2,1X,I2)') UNIT(I,1),UNIT(I,2)
        DO 20 M=1, (NTYP1-1)
          IF (UNIT(I,1) .EQ. M) MUNIT(M) = MUNIT(M) + 1
20      CONTINUE
        IF (UNIT(I,1) .NE. 0) MUNIT(NTYP1) = MUNIT(NTYP1)+1
30    CONTINUE
      DO 40 I=1, NSTRM
        READ (14,'(1X,I2,1X,I2)') STREAM(I,1), STREAM(I,2)
40    CONTINUE
      DO 50 I=1, NCONN
        READ (14,'(1X,I2,1X,I2)') CONN(I,1), CONN(I,2)
50    CONTINUE
      CLOSE (UNIT=14)

C           Specify indices for starting positions in vectors:
C           - X contains only the mols of all components in each unit with holdup.
```

```
C               - A contains the total number of mols, the total volume and the liquid volume in each unit
C                 with holdup, the number of mols of each component, the total number of mols and the
C                 total volume in each of the streams.
      INX(1) = 0
      INA(1) = 0
      DO 60 I=2,NUNIT
       LU0 = UNIT(I-1,1)
       IF ((LU0 .EQ. 1) .OR. (LU0 .EQ. 2) .OR. (LU0 .EQ. 5) .OR.
     &   (LU0 .EQ. 6) .OR. (LU0 .EQ. 7)) THEN
C                                                    assign space in X and A only for units with holdup
        INX(I) = INX(I-1) + NCOMP
        INA(I) = INA(I-1) + NTOTS
       ELSE
        INX(I) = INX(I-1)
        INA(I) = INA(I-1)
       ENDIF
60    CONTINUE
      DO 70 I=1,NSTRM
       INA(NUNIT+I) = NUNIT*NTOTS + (I-1)*(NCOMP+NTOTS)
70    CONTINUE
      DO 80 I=1,NCONN
       INA(NUNIT+NSTRM+I) = NUNIT*NTOTS + NSTRM*(NCOMP+
     &                              NTOTS) + (I-1)*2
80    CONTINUE

C                                                    read in densities and molar masses
      OPEN (16, FILE='phys.dat')
      DO 100 M=1,NTYP2
       DO 90 J=1,NCOMP
        READ (16,'(F7.3,2X,F7.3)') PHYS(M,J,1),PHYS(M,J,2)
        IF (PHYS(M,J,2) .NE. 0.0) THEN
         PHYS(M,J,2) = PHYS(M,J,2)*1000.0
C                                                    => PHYS(2) units of kg/m3
         CONV(M,J) = PHYS(M,J,1)/PHYS(M,J,2)
C                                                    CONV has units of m3/kmol
        ELSE
         CONV(M,J) = ZERO
        ENDIF
90     CONTINUE
100   CONTINUE
      CLOSE (16)
C                                                    read stoichiometric constants from file
      OPEN (17, FILE='chem.dat')
      DO 110 J=1,NCOMP
       READ (17,5) STOI(1,J,1),STOI(1,J,2),STOI(1,J,3),STOI(1,J,4),
     & STOI(1,J,5),STOI(1,J,6),STOI(1,J,7),STOI(1,J,8),STOI(1,J,9),
     & STOI(1,J,10),STOI(1,J,11),STOI(1,J,12)
110   CONTINUE
      READ (17,25) RK(1,1),RK(1,2),RK(1,3),RK(1,4),RK(1,5),RK(1,6),
     &       RK(1,7),RK(1,8),RK(1,9),RK(1,10),RK(1,11),RK(1,12)
      DO 120 J=1,NCOMP
       READ (17,15) STOI(2,J,1),STOI(2,J,2),STOI(2,J,3),STOI(2,J,4),
     & STOI(2,J,5),STOI(2,J,6),STOI(2,J,7),STOI(2,J,8),STOI(2,J,9),
     & STOI(2,J,10),STOI(2,J,11),STOI(2,J,12)
120   CONTINUE
      READ (17,25) RK(2,1),RK(2,2),RK(2,3),RK(2,4),RK(2,5),RK(2,6),
     &       RK(2,7),RK(2,8),RK(2,9),RK(2,10),RK(2,11),RK(2,12)
      CLOSE (17)
C                                                    initially set all variables equal to zero
      DO 130 I=1,NSTAT
       X(I) = ZERO
130   CONTINUE
      DO 140 I=1,NALGB
       A(I) = ZERO
140   CONTINUE
C                                                    integration constants
      DT = 60.0
```

```
      H1 = 1.0
      TT = ZERO
      HMIN = 1.0E-4
      D = 5.0E+7
      EPS = 5.0E-6
      DTSAV = 600.0
      TSAV = -1.1*DTSAV
      TSAV2 = ZERO
      KOUNT = 0
      NBAD = 0
      NOK = 0
      KALLS = 0
      KALLS2 = 0
      LUAT = 0
      KROUND = 0
      NCOND2 = 0
      NCOLL = 0
      N1 = 0
      VTNK = 6.0*PI*(7.0/2)**2
      VSCR = 0.7*PI*(3.9/2)**2
      CALL COLLECT (X,NSTAT,A,NALGB,NT,GOLD,AUCN,NCOLL)

      DO 150 M=1,NSTRM
        FLO(M) = ZERO
150   CONTINUE

      PRINT *,'Would you like to :'
      PRINT *,'(1): Start the simulation with empty tanks and constant',
     &     ' flows'
      PRINT *,' 2 : Start the simulation where the last has ended off',
     &     ' again with'
      PRINT *,'     constant flows, or'
      PRINT *,' 3 : Use steady-state data as IC's with plant data ?'
      OPTSIM = '1'
160   READ (*,'(A)') OPTSIM
      IF ((OPTSIM .NE. '1') .AND. (OPTSIM .NE. '2') .AND.
     &  (OPTSIM .NE. '3')) THEN
        PRINT *,'Please choose option 1,2 or 3'
        GOTO 160
      ELSE
        OPEN (18, FILE = 'inflos.pdt')

        IF (OPTSIM .EQ. '1') THEN
          PRINT *,'How long is the simulation to run for (in minutes) ?'
          READ (*,'(I6)') NT
          TE = NT*60.0
          T1 = ZERO
          T2 = T1 + DT
C                                                    read in data for feed units
          VOL = 3.5*3.5*PI*5.3
          PRINT *,'Is the Carbon profile to be :'
          PRINT *,'(1): Smooth ?'
          PRINT *,' 2 : Weighted to the top ?'
          PRINT *,' 3 : Weighted to the bottom ?'
          OPT1 = '1'
170       READ (*,'(A)') OPT1
          IF ((OPT1.NE.'1') .AND. (OPT1.NE.'2') .AND. (OPT1.NE.'3'))
     &    THEN
            PRINT *,'Please choose one of these options.'
            GOTO 170
          ENDIF
          DO 180 L=1,NUNIT
            LU1 = UNIT(L,1)
            IF (LU1 .EQ. 1) THEN
              READ (18,35) X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &       X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &       X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
```

```
     &     X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &     X(INX(L)+16),X(INX(L)+17),X(INX(L)+18)
           ELSEIF (LU1 .EQ. 7) THEN
            HLA(L) = 1.0
            HLD(L) = 0.0
            IBLK(L) = 0
C                                                          add coarse carbon to CIP tanks only
            IF (OPT1 .EQ. '1') THEN
C                                                          all tanks contain 2% C by volume
             X(INX(L)+7) = VOL*0.02/CONV(2,7)
            ELSEIF (OPT1 .EQ. '2') THEN
             IF ((L.EQ.18) .OR. (L.EQ.21) .OR. (L.EQ.22)) THEN
C                                                          the first three tanks contain 3% C by volume
              X(INX(L)+7) = VOL*0.03/CONV(2,7)
             ELSE
              X(INX(L)+7) = VOL*0.02/CONV(2,7)
             ENDIF
            ELSE
             IF ((L .EQ. 25) .OR. (L .EQ. 26) .OR. (L .EQ. 28)) THEN
C                                                          the last three tanks contain 3% C by volume
              X(INX(L)+7) = VOL*0.03/CONV(2,7)
             ELSE
              X(INX(L)+7) = VOL*0.02/CONV(2,7)
             ENDIF
            ENDIF
           ENDIF
180       CONTINUE

          ELSEIF (OPTSIM .EQ. '2') THEN
           PRINT *,'How long is the simulation to run for (in minutes) ?'
           READ (*,'(I6)') NT
           OPEN (19, FILE = 'psdata.pdt')
           DO 200 L=1,NUNIT
            LU1 = UNIT(L,1)
            IF (LU1 .EQ. 1) THEN
             READ (18,35) X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &     X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &     X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
     &     X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &     X(INX(L)+16),X(INX(L)+17),X(INX(L)+18)
            ELSEIF ((LU1 .EQ. 2) .OR. (LU1 .EQ. 5) .OR. (LU1.EQ.6) .OR.
     &          (LU1 .EQ. 7)) THEN
             READ (19,45) TE,X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &     X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &     X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
     &     X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &     X(INX(L)+16),X(INX(L)+17),X(INX(L)+18),TT
             tsav2 = te
             IF (LU1 .EQ. 2) THEN
              IF ((L .EQ. 20) .AND. (X(INX(L)+18) .GT. 5.0)) THEN
               FLO(18) = 1.0
              ENDIF
             ELSEIF (LU1 .EQ. 7) THEN
              HLA(L) = 1.0
              HLD(L) = 0.0
              IBLK(L) = 0
C                                                          recognise engaged transfer stream
              IF (X(INX(L)+18) .GT. 5.0) THEN
               DO 190 M=1,NSTRM
                IF ((STREAM(M,2) .EQ. L) .AND.
     &           (STREAM(M+1,2) .EQ. STREAM(M,1))) THEN
                  FLO(M) = 1.0
                ENDIF
190            CONTINUE
               IF (L .EQ. 28) THEN
                FLO(35) = 1.0
               ENDIF
```

```
            ENDIF
           ENDIF
          ENDIF
200       CONTINUE
          T1 = TE
          TE = NT*60.0 + T1
          T2 = T1 + DT
          CLOSE (19)
         ELSE
C                                                          for OPTSIM equal to 3 :
          OPEN (18, FILE = 'inflos.pdt')
          OPEN (19, FILE = 'ssdata.pdt')
          DO 220 L=1,NUNIT
           LU1 = UNIT(L,1)
           IF (LU1 .EQ. 1) THEN
            READ (18,35) X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &     X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &     X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
     &     X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &     X(INX(L)+16),X(INX(L)+17),X(INX(L)+18)
           ELSEIF ((LU1 .EQ. 2) .OR. (LU1 .EQ. 5) .OR. (LU1.EQ. 6).OR.
     &          (LU1 .EQ. 7)) THEN
            READ (19,45) TE,X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &     X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &     X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
     &     X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &     X(INX(L)+16),X(INX(L)+17),X(INX(L)+18),TT
            IF (LU1 .EQ. 2) THEN
             IF ((L .EQ. 20) .AND. (X(INX(L)+18).GT.5.0)) THEN
              FLO(18) = 1.0
              print *,'started transfer stream 18'
             ENDIF
            ELSEIF (LU1 .EQ. 7) THEN
             HLA(L) = 1.0
             HLD(L) = 0.0
             IBLK(L) = 0
C                                                          recognise engaged transfer stream
             IF (X(INX(L)+18) .GT. 5.0) THEN
              DO 210 M=1,NSTRM
               IF ((STREAM(M,2) .EQ. L) .AND.
     &          (STREAM(M+1,2) .EQ. STREAM(M,1))) THEN
                FLO(M) = 1.0
                print *,'started transfer stream',M
               ENDIF
210           CONTINUE
              IF (L .EQ. 28) THEN
               FLO(35) = 1.0
               print *,'started transfer stream 35'
              ENDIF
             ENDIF
            ENDIF
           ENDIF
220       CONTINUE
          CLOSE (18)
          CLOSE (19)
          TT = TT - TE
          TE = ZERO
         ENDIF
         CLOSE (18)

         CALL OPTIONS
         PRINT *,' Time    ScrT Vol   L10 Vol    CIP8 Vol',
     &        '   Lch eff   CIP eff   Fnc Calls'
         IF ((OPTSIM .EQ. '1') .OR. (OPTSIM .EQ.'2')) GOTO 260
         OPEN(31, FILE = 'av12_0.pdt')
         OPEN(32, FILE = 'abs2_0.pdt')
         OPEN(33, FILE = 'abs3_0.pdt')
```

```
        OPEN(34, FILE = 'av23_0.pdt')
       ENDIF

230    READ(31,55) MT,DAT(1),DAT(2),DAT(3),DAT(4),DAT(5),DAT(6),DAT(7),
     &          DAT(8),DAT(9)
C                       plant data is read in here: dat(1) : CN-flow
C                       dat(2) : thick2-flow            dat(3) : thick2-fl-sp
C                       dat(4) : conductivity           dat(5) : conduct-sp
C                       dat(6) : CIP-feed     dat(7) : leach-feed
C                       dat(8) : leach-fd-sp            dat(9) : leach-densty
       READ(32,65) MT,DAT(10),DAT(11),DAT(12),DAT(13),DAT(14),DAT(15),
     &          DAT(16),DAT(17),DAT(18)
       IF (DAT(16) .EQ. 0.0) THEN
        LUAT = 0
       ELSE
        LUAT = 1
       ENDIF
C                       dat(10) : lime lvl              dat(11) : caustic lvl
C                       dat(12) : elu.CN.lvl            dat(13) : lch.CN.lvl1
C                       dat(14) : lch.CN.lvl2           dat(15) : elu.p 1
C                       dat(16) : eluat p2              dat(17) : sump 1
C                       dat(18) : sump 2
       IF (OPT9 .EQ. '3') THEN
        FLO1(18) = FLO(18)
        FLO1(21) = FLO(21)
        FLO1(23) = FLO(23)
        FLO1(25) = FLO(25)
        FLO1(27) = FLO(27)
        FLO1(29) = FLO(29)
        FLO1(31) = FLO(31)
        FLO1(33) = FLO(33)
        FLO1(35) = FLO(35)
        READ(33,75) MT,FLO(18),FLO(21),FLO(23),FLO(25),FLO(27),FLO(29),
     &          FLO(31),FLO(33),CLO
C                               flo(19) : C trans 1             flo(21) : C trans 2
C                               flo(23) : C trans 3             flo(25) : C trans 4
C                               flo(27) : C trans 5             flo(29) : C trans 6
C                               flo(31) : C trans 7             flo(33) : C trans 8
C                               clo     : C leak
        IF (FLO(33) .GT. ZERO) THEN
         FLO(35) = 1.0
        ELSE
         FLO(35) = ZERO
        ENDIF
        IF (FLO1(18) .EQ. 1.0) THEN
         IF (FLO(18) .NE. 1.0) THEN
          PRINT *,'Stopped transfer stream       18'
          X(INX(20)+18) = 0.1
         ENDIF
        ELSE
         IF (FLO(18) .NE. ZERO) PRINT *,'Started transfer stream    18'
        ENDIF
        DO 240 N=1,8
         IF (FLO1(N*2+19) .EQ. 1.0) THEN
          IF (FLO(N*2+19) .NE. 1.0) THEN
           PRINT *,'Stopped transfer stream ',(N*2+19)
           X(INX(STREAM(N*2+19,2))+18) = 0.1
          ENDIF
         ELSE
          IF (FLO(N*2+19) .NE. ZERO) THEN
           PRINT *,'Started transfer stream ',(N*2+19)
          ENDIF
         ENDIF
240      CONTINUE
       ENDIF

c      READ(34,75) MT,HLA(18),HLA(21),HLA(22),HLA(23),HLA(24),HLA(25),
```

```
c     &          HLA(26),HLA(28)
C                                  hla(18) : hilvl alm1        hla(21) : hilvl alm2
C                                  hla(22) : hilvl alm3        hla(23) : hilvl alm4
C                                  hla(24) : hilvl alm5        hla(25) : hilvl alm6
C                                  hla(26) : hilvl alm7        hla(28) : hilvl alm8
      T1 = TE
      T2 = T1 + DT
      TE = 60.0*MT
      KROUND = 0
      H1 = 15.0

250   CONTINUE
C                                                                          screen blockage :
C                                                  remove c's if screen blockage is to be included in simulation
c       IF ((T2 .GT.  5400.0*60.0) .AND. (N1 .EQ. 0)) THEN
c         N1 = 1
c         HLA(18) = 0.0
c       ENDIF

        DO 260 M=1,NUNIT
         IF (UNIT(M,1) .EQ. 7) THEN
          IF (IBLK(M) .EQ. 0) THEN
           IF (HLA(M) .EQ. 0.0) THEN
            IF (HLD(M) .EQ. 0.0) THEN
             HLD(M) = 1.0
            ELSE
             HLD(M) = 2.0
             print *,'Screen blocked in tank ',M
             IBLK(M) = 1
            ENDIF
           ELSE
            IF (HLD(M) .EQ. 1.0) HLD(M) = 0.0
           ENDIF
          ELSEIF (IBLK(M) .EQ. 1) THEN
           print *,'vol =',A(INA(M)+2),'  vtnk=',VTNK
           IF (A(INA(M)+2) .GE. (VTNK)) THEN
            IBLK(M) = 2
            print *,'Screen overflowed in tank ',M
           ENDIF
          ELSE
           IF (A(INA(M)+2) .LE. (VTNK-VSCR)) THEN
            print *,'Screen unblocked in tank ',M
            IBLK(M) = 0
            HLA(M) = 1.0
            HLD(M) = 0.0
           ENDIF
          ENDIF
         ENDIF
260     CONTINUE

        CALL ODEINT(X,NSTAT,A,NALGB,T1,T2,H1,HMIN,D,EPS,NOK,NBAD,
     & DERIVS,BSSTEP)
        NT = T2/60

        OPEN (37, FILE = 'store.dat')
C                                                                  save state variables after each step
        DO 270 L=1,NUNIT
         LU1 = UNIT(L,1)
         IF ((LU1.EQ.2).OR.(LU1.EQ.5).OR.(LU1.EQ.6).OR.(LU1.EQ.7)) THEN
          WRITE (37,45) T2,X(INX(L)+1),X(INX(L)+2),X(INX(L)+3),
     &    X(INX(L)+4),X(INX(L)+5),X(INX(L)+6),X(INX(L)+7),
     &    X(INX(L)+8),X(INX(L)+9),X(INX(L)+10),X(INX(L)+11),
     &    X(INX(L)+12),X(INX(L)+13),X(INX(L)+14),X(INX(L)+15),
     &    X(INX(L)+16),X(INX(L)+17),X(INX(L)+18),TT
         ENDIF
270     CONTINUE
        CLOSE (37)
```

```
      IF ((T2-TSAV2) .GE. DTSAV) THEN
       NT = T2/60
       TSAV2 = T2
       GOLD = (X(INX(3)+8)+X(INX(3)+9))/(100.0*X(INX(3)+2)+TINY)
       AUCN = X(INX(16)+5)/(100.0*X(INX(16)+1)+TINY)
       WRITE (*,115) NT,A(INA(3)+2),A(INA(16)+2),A(INA(28)+2),
     &  (X(INX(16)+8)+X(INX(16)+9))/(GOLD*X(INX(16)+2)+TINY),
     &   X(INX(28)+5)/(AUCN*X(INX(28)+1)+TINY),KALLS2,KALLS
       CALL COLLECT(X,XSTAT,A,NALGB,NT,GOLD,AUCN,NCOLL)
      ENDIF

      KOUNT = 0

C                                                          regular carbon transfers :
C                                                        set maximum C-conc for top-ups
      CCLIMIT = 0.02*3.5*3.5*PI*5.3/CONV(2,7)
C                                                              set the size of transfer
      IF (OPT3 .EQ. '1') THEN
       TRLIMIT = 5000.0/PHYS(2,7,1)
      ELSE
       TRLIMIT = 2500.0/PHYS(2,7,1)
      ENDIF
C                                                          set beginning time of transfer
      IF (OPT9 .EQ. '1') THEN
       HR = 16.0
      ELSEIF (OPT9 .EQ. '2') THEN
       HR = 8.0
      ENDIF

      IF ((OPT9.NE.'3') .AND. (X(INX(29)+1).GT.ZERO)) THEN
C                                                start transfers if not using data and whole cascade is full
       IF ((OPT4.EQ.'0') .OR.((OPT4.EQ.'1') .AND.(NCOND2.EQ.0))) THEN
        IF ((TT .EQ. ZERO) .OR. ((T2-TT) .GE. HR*3600.0)) THEN
C                                       start only if its the 1st time or HR hr passed since previous one
         IF ((OPT2 .EQ. '1') .OR. (OPT2.EQ.'3') .OR. (OPT2.EQ.'4'))
     &    THEN
           DO 280 M=1,NSTRM
C                                          for simultaneous and continuous transfers start all transfers
            IF ((STREAM(M,1) .NE. 0) .AND. (FLO(M) .EQ. ZERO)) THEN
             IF ((STREAM(M,1) .EQ. STREAM(M+1,2)) .AND.
     &       (STREAM(M,2) .EQ. STREAM(M+1,1))) THEN
               FLO(M) = 1.0
               print *,'starting transfer stream',m
             ENDIF
             IF (STREAM(M,1) .EQ. 27) THEN
              FLO(M) = 1.0
              print *,'starting transfer stream',m
              KROUND = 0
             ENDIF
            ENDIF
280         CONTINUE
           ELSEIF ((OPT2.EQ.'2') .OR. (OPT2.EQ.'5')) THEN
C                                          for consecutive transfer scheme start only first transfer
            FLO(18) = 1.0
            PRINT *,'Starting transfer stream        18'
           ENDIF
           TT = T2
          ENDIF
          IF (OPT2 .NE. '3') THEN
C                                                for continuous transfer scheme don't stop streams
           DO 310 M=1,NSTRM
            IF (FLO(M) .EQ. 1.0) THEN
             IF (STREAM(M,2) .EQ. 19) THEN
              IF (X(INX(20)+18) .GE. TRLIMIT) THEN
               FLO(M) = ZERO
               PRINT *,'stopped transfer stream',m
               X(INX(20)+18) = X(INX(20)+18) - TRLIMIT
```

```
                IF ((OPT2.EQ.'2') .OR. (OPT2.EQ.'5')) THEN
C                                                          only for consecutive transfer start next stream
                 DO 290 N=1,NSTRM
                  IF ((STREAM(N,2) .EQ. STREAM(M,1)) .AND.
     &            (STREAM(N,1) .EQ. STREAM(N+1,2))) THEN
                    FLO(N) = 1.0
                    PRINT *,'started transfer stream',n
                  ENDIF
290               CONTINUE
                 ENDIF
                ENDIF
               ELSE
                IF (X(INX(STREAM(M,2))+18) .GE. TRLIMIT) THEN
                 FLO(M) = ZERO
                 print *,'stopping transfer stream',m
                 NST = STREAM(M,2)
                 X(INX(NST)+18) = X(INX(NST)+18) - TRLIMIT
                 IF (STREAM(M,1) .EQ. 27) THEN
                  KROUND = 0
                  NCOND1 = 1
                 ENDIF
                 IF ((OPT2.EQ.'2').OR.(OPT2.EQ.'5')) THEN
C                                                          only for consecutive transfer start next stream
                  IF (STREAM(M,1) .EQ. 28) THEN
                   FLO(35) = 1.0
                   PRINT *,'started transfer stream 35'
                   KROUND = 0
                  ELSE
                   DO 300 N=1,NSTRM
                    IF ((STREAM(N,2) .EQ. STREAM(M,1)) .AND.
     &              (STREAM(N,1) .EQ. STREAM(N+1,2))) THEN
                      FLO(N) = 1.0
                      PRINT *,'started transfer stream',n
                    ENDIF
300                 CONTINUE
                   ENDIF
                  ENDIF
                 ENDIF
                ENDIF
               ENDIF
310           CONTINUE
              END
C                                                          decide whether it is time for a top-up
              NOFLO = 0
              DO 320 M=1,NSTRM
               IF (FLO(M) .EQ. 1.0) NOFLO = 1
320           CONTINUE
C                                          conditions are needed to ensure only one top-up after each transfer
              IF ((NOFLO .EQ. 0) .AND. (NCOND1 .EQ. 1)) THEN
               NCOND2 = 1
              ENDIF
             ELSE
C                                                          top-up tanks sequentially from top tank down
              DO 340 M=1,NSTRM
               IF (FLO(M) .EQ. ZERO) THEN
                IF ((STREAM(M,2) .EQ. 18) .AND. (NCOND1 .EQ.1)) THEN
                 IF (X(INX(STREAM(M,2))+7) .LT. CCLIMIT) THEN
                  FLO(21) = 1.0
                  PRINT *,'topping up tank ',STREAM(M,2)
                 ELSE
                  NCOND2 = 0
C                                                          if the first tank needs no topup, leave others as well
                 ENDIF
                 NCOND1 = 0
                ENDIF
               ELSE
                IF (X(INX(STREAM(M,2))+7) .GE. CCLIMIT) THEN
```

```
                FLO(M) = zero
                NST = STREAM(M,2)
                PRINT *,'stopped topping up tank ',NST
                X(INX(STREAM(M,2))+18) = 0.1
                IF (STREAM(M,1) .EQ. 27) THEN
                  KROUND = 0
                  NCOND2 = 0
                ELSEIF (STREAM(M,1) .EQ. 28) THEN
                  FLO(35) = 1.0
                  PRINT *,'started topping up tank ',STREAM(M,1)
                  KROUND = 0
                ELSE
                  DO 330 N=1,NSTRM
                    IF ((STREAM(N,2) .EQ. STREAM(M,1)) .AND.
     &             (STREAM(N,1) .EQ. STREAM(N+1,2))) THEN
                      FLO(N) = 1.0
                      PRINT *,'started topping up tank ',STREAM(N,2)
                    ENDIF
330                 CONTINUE
                  ENDIF
                ENDIF
              ENDIF
340         CONTINUE
            ENDIF
          ENDIF

          IF (T2 .LT. TE) THEN
            T1 = T2
            T2 = T2 + DT
            IF (T2 .GT. TE) T2 = TE
            GOTO 250
          ENDIF

          IF (OPTSIM .EQ. '3') THEN
            IF (TE .LT. 604800.0) THEN
              GOTO 230
            ELSE
              CLOSE (31)
              CLOSE (32)
              CLOSE (33)
              CLOSE (34)
            ENDIF
          ENDIF

          NCOLL = 2
          CALL COLLECT(X,NSTAT,A,NALGB,NT,GOLD,AUCN,NCOLL)

          STOP
          END

C ***************************************************************************
C                                                                           *
          SUBROUTINE OPTIONS
C                                                                           *
C         This subroutine asks the user for his choice in simulating        *
C         various different prespecified options.                           *
C                                                                           *
C ***************************************************************************

          DOUBLE PRECISION TRLIMIT,CCLIMIT
          COMMON /FEEDS/ OPTSIM,DAT(18),LUAT
          COMMON /OPTNS/ OPT2,OPT3,TRLIMIT,OPT4,CCLIMIT,NCOND2,OPT5,
     &           OPT6,OPT7,OPT8,OPT9
          CHARACTER ANS

          PRINT *,'Would you like the Carbon Transfers to be :'
          PRINT *,'(1): Equal and simultaneous ?'
```

```
      PRINT *,' 2 : Equal and consecutive ?'
      PRINT *,' 3 : Equal and continuous ?'
      PRINT *,' 4 : Plant flowrates and simultaneous'
      PRINT *,' 5 : Plant flowrates and consecutive'
      OPT2 = '1'
10    READ (*,'(A)') OPT2
      IF ((OPT2.NE.'1') .AND. (OPT2.NE.'2') .AND. (OPT2.NE.'3')
     &  .AND. (OPT2.NE.'4') .AND. (OPT2.NE.'5')) THEN
       PRINT *,'Please choose one of the available options.'
       GOTO 10
      ENDIF

      IF (OPT2 .NE. '3') THEN

       PRINT *,'Should the Transfers start :'
       PRINT *,'(1): Regularly every 16hr ?'
       PRINT *,' 2 : Regularly every 8hr ?'
       IF ((OPTSIM .EQ. '1') .OR. (OPTSIM .EQ. '2')) THEN
20       READ (*,'(A)') OPT9
         IF ((OPT9.NE.'1') .AND. (OPT9.NE.'2')) THEN
           PRINT *,'Please choose one of the available options.'
           GOTO 20
         ENDIF
       ELSE
         PRINT *,' 3 : As recorded on the plant ?'
         OPT9 = '1'
30       READ (*,'(A)') OPT9
         IF ((OPT9.NE.'1') .AND.(OPT9.NE.'2') .AND. (OPT9.NE.'3')) THEN
           PRINT *,'Please choose either option 1, 2 or 3.'
           GOTO 30
         ENDIF
       ENDIF

       PRINT *,'And should the Transfers be :'
       PRINT *,'(1): Large (5000kg) ?'
       PRINT *,' 2 : Small (2500kg) ?'
       OPT3 = '1'
40     READ (*,'(A)') OPT3
       IF ((OPT3 .NE. '1') .AND. (OPT3 .NE. '2')) THEN
         PRINT *,'Please choose either option 1 or 2.'
         GOTO 40
       ENDIF

       PRINT *,'Should the amount of Carbon be topped up after',
     &       'transfers [(Y) or N] ?'
       ANS = 'Y'
50     READ (*,'(A)') ANS
       IF ((ANS .EQ. 'y') .OR. (ANS .EQ. 'Y')) OPT4 = '1'
       IF ((ANS .EQ. 'n') .OR. (ANS .EQ. 'N')) OPT4 = '0'
       IF ((OPT4.NE.'1') .AND. (OPT4.NE.'0')) THEN
         PRINT *,'Please choose either Y or N'
         GOTO 50
       ENDIF
      ELSE
       PRINT *,'And should the Transfers be :'
       PRINT *,'(1): Large (5000kg every 16hr) ?'
       PRINT *,' 2 : Small (2500kg every 16hr) ?'
       OPT3 = '1'
60     READ (*,'(A)') OPT3
       IF ((OPT3 .NE. '1') .AND. (OPT3 .NE. '2')) THEN
         PRINT *,'Please choose either option 1 or 2.'
         GOTO 60
       ENDIF
       OPT4 = '0'
      ENDIF

      PRINT *,'Is Carbon allowed to leak through the screens',
```

```
     &       '[(Y) or N] ?'
          ANS = 'Y'
70        READ (*,'(A)') ANS
          IF ((ANS .EQ. 'y') .OR. (ANS .EQ. 'Y')) OPT5 = '1'
          IF ((ANS .EQ. 'n') .OR. (ANS .EQ. 'N')) OPT5 = '0'
          IF ((OPT5.NE.'1') .AND. (OPT5.NE.'0')) THEN
           PRINT *,'Please choose either Y or N'
           GOTO 70
          ENDIF

          IF (OPTSIM .EQ. '3') THEN
           PRINT *,'Is the pulp flow to be:'
           PRINT *,'(1) : Constant ?'
           PRINT *,' 2  : As recorded in the plant data ?'
           OPT6 = '1'
80         READ (*,'(A)') OPT6
           IF ((OPT6 .NE. '1') .AND. (OPT6 .NE. '2')) THEN
            PRINT *,'Please choose either option 1 or 2.'
            GOTO 80
           ENDIF

           IF (OPT6 .EQ. '2') THEN
            PRINT *,'Is the lime addition to be:'
            PRINT *,'(1) : Constant ?'
            PRINT *,' 2  : Proportional to the recorded flow ?'
            OPT7 = '1'
90          READ (*,'(A)') OPT7
            IF ((OPT7 .NE. '1') .AND. (OPT7 .NE. '2')) THEN
             PRINT *,'Please choose either option 1 or 2.'
             GOTO 90
            ENDIF

            PRINT *,'Is the cyanide addition to be:'
            PRINT *,'(1) : Constant ?'
            PRINT *,' 2  : Proportional to the recorded flow ?'
            PRINT *,' 3  : As recorded in the plant data ?'
            OPT8 = '1'
100         READ (*,'(A)') OPT8
            IF ((OPT8.NE.'1').AND.(OPT8.NE.'2').AND.(OPT8.NE.'3')) THEN
             PRINT *,'Please choose either option 1,2 or 3.'
             GOTO 100
            ENDIF
           ELSE
            OPT7 = '1'
            OPT8 = '1'
           ENDIF
          ENDIF

          RETURN
          END

C ***************************************************************************
C                                                                           *
          SUBROUTINE COLLECT(X,NS,A,NA,NT,GOLD,AUCN,NCOLL)
C                                                                           *
C         This subroutine writes the required data to file.                 *
C                                                                           *
C ***************************************************************************

          PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
          PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2,  NREAC = 12)
          PARAMETER (KMAX  = 10)
          PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                     + NCONN*2)
          PARAMETER (NSTAT = NUNIT*NCOMP)
          PARAMETER (NPROC = NUNIT + NSTRM + NCONN)
```

```
      DOUBLE PRECISION X,A,TT,ZERO,CONV,VOL,GOLD,AUCN
      INTEGER UNIT, STREAM, CONN

      PARAMETER (ZERO = 0.0, TINY=1.0E-30)
      DIMENSION X(NSTAT),A(NALGB)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),CONN(NCONN,2),
     &        INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /FEEDS/ OPTSIM,DAT(18),LUAT

5     FORMAT (I6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &   E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &   E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,E11.6,1X,
     &   E11.6,1X,E11.6,1X,E11.6,1X,E11.6)
15    FORMAT (I8,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,
     &   F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,
     &   F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,
     &   F8.3)
      IF (NCOLL .EQ. 0) THEN
       NCOLL = 1
       OPEN (36, FILE = 'outflos.sim')
       OPEN (21, FILE = 'solgold.sim')
       OPEN (22, FILE = 'disgold.sim')
       OPEN (23, FILE = 'adsgold.sim')
       OPEN (24, FILE = 'solmetl.sim')
       OPEN (26, FILE = 'dismetl.sim')
       OPEN (27, FILE = 'adsmetl.sim')
       OPEN (28, FILE = 'cyanide.sim')
       OPEN (29, FILE = 'disoxyg.sim')
       OPEN (38, FILE = 'carbtrn.sim')
       OPEN (39, FILE = 'sollime.sim')
       OPEN (41, FILE = 'carbonp.sim')
       OPEN (42, FILE = 'effncy.sim')
       OPEN (43, FILE = 'leffcy.sim')

      ELSEIF (NCOLL .EQ. 1) THEN
C                                                    save volume flows out of selected tanks
       IF (OPTSIM .EQ. '3') THEN
        WRITE (36,15) NT,DAT(7),
     &          A(INA(NUNIT+3)+NCOMP+2)*3600,
     &          A(INA(NUNIT+6)+NCOMP+2)*3600,
     &          A(INA(NUNIT+7)+NCOMP+2)*3600,
     &          A(INA(NUNIT+8)+NCOMP+2)*3600,
     &          A(INA(NUNIT+9)+NCOMP+2)*3600,
     &          A(INA(NUNIT+10)+NCOMP+2)*3600,
     &          A(INA(NUNIT+11)+NCOMP+2)*3600,
     &          A(INA(NUNIT+12)+NCOMP+2)*3600,
     &          A(INA(NUNIT+13)+NCOMP+2)*3600,
     &          A(INA(NUNIT+14)+NCOMP+2)*3600,DAT(6)
       ELSE
        WRITE (36,15) NT,
     &          A(INA(NUNIT+1)+NCOMP+2)*3600,
     &          A(INA(NUNIT+6)+NCOMP+2)*3600,
     &          A(INA(NUNIT+7)+NCOMP+2)*3600,
     &          A(INA(NUNIT+8)+NCOMP+2)*3600,
     &          A(INA(NUNIT+9)+NCOMP+2)*3600,
     &          A(INA(NUNIT+10)+NCOMP+2)*3600,
     &          A(INA(NUNIT+11)+NCOMP+2)*3600,
     &          A(INA(NUNIT+12)+NCOMP+2)*3600,
     &          A(INA(NUNIT+13)+NCOMP+2)*3600,
     &          A(INA(NUNIT+14)+NCOMP+2)*3600,
     &          A(INA(NUNIT+15)+NCOMP+2)*3600,
     &          A(INA(NUNIT+16)+NCOMP+2)*3600,
     &          A(INA(NUNIT+17)+NCOMP+2)*3600,
     &          A(INA(NUNIT+22)+NCOMP+2)*3600,
     &          A(INA(NUNIT+24)+NCOMP+2)*3600,
```

```
     &              A(INA(NUNIT+26)+NCOMP+2)*3600,
     &              A(INA(NUNIT+28)+NCOMP+2)*3600,
     &              A(INA(NUNIT+30)+NCOMP+2)*3600,
     &              A(INA(NUNIT+32)+NCOMP+2)*3600,
     &              A(INA(NUNIT+34)+NCOMP+2)*3600,
     &              A(INA(NUNIT+34)+NCOMP+2)*3600
          ENDIF
C                                                          save normalized solid conc of gold
          WRITE (21,5) NT,
     &   (X(INX(7)+8)+X(INX(7)+9))/(GOLD*(X(INX(7)+2)+TINY)),
     &   (X(INX(8)+8)+X(INX(8)+9))/(GOLD*(X(INX(8)+2)+TINY)),
     &   (X(INX(9)+8)+X(INX(9)+9))/(GOLD*(X(INX(9)+2)+TINY)),
     &   (X(INX(10)+8)+X(INX(10)+9))/(GOLD*(X(INX(10)+2)+TINY)),
     &   (X(INX(11)+8)+X(INX(11)+9))/(GOLD*(X(INX(11)+2)+TINY)),
     &   (X(INX(12)+8)+X(INX(12)+9))/(GOLD*(X(INX(12)+2)+TINY)),
     &   (X(INX(13)+8)+X(INX(13)+9))/(GOLD*(X(INX(13)+2)+TINY)),
     &   (X(INX(14)+8)+X(INX(14)+9))/(GOLD*(X(INX(14)+2)+TINY)),
     &   (X(INX(15)+8)+X(INX(15)+9))/(GOLD*(X(INX(15)+2)+TINY)),
     &   (X(INX(16)+8)+X(INX(16)+9))/(GOLD*(X(INX(16)+2)+TINY))
                :                 :
                :                 :
            (a few pages of WRITE statements are omitted here)
                :                 :
                :                 :
          ELSE
           CLOSE (21)
           CLOSE (22)
           CLOSE (23)
           CLOSE (24)
           CLOSE (26)
           CLOSE (27)
           CLOSE (28)
           CLOSE (29)
           CLOSE (36)
           CLOSE (38)
           CLOSE (39)
           CLOSE (41)
           CLOSE (42)
          ENDIF
          RETURN
          END
C ***************************************************************************
C                                                                            *
C    Copyright (c) MINTEK 1991. Right of Reproduction Reserved.              *
C                                                                            *
C ***************************************************************************
```

I.2 BSINT.F : INTEGRATION SUBROUTINE

```
C ***************************************************************************
C                                                                            *
          SUBROUTINE ODEINT(XSTART,NS,A,NA,T1,T2,H1,HMIN,D,EPS,NOK,
     *NBAD,DERIVS,BSSTEP)
C                                                                            *
C         This integration  package uses the  Bulirsch-Stoer  method with    *
C         adaptive stepsize control as given by W.H.Press et.al. in their    *
C         book 'Numerical Recipes: The Art of Scientific Computing', Cam-    *
C         bridge University Press,1986. It has been modified to deal with    *
C         discontinuities, using the method supplied by Gear C.W. and Øs-    *
C         terby O, Solving Ordinary Differential Equations with Disconti-    *
C         nuities, ACM Trans. on Math. Software, Vol 10, No.1, 1984.         *
C                                                                            *
C         The following (in CAPITALS) must be supplied:                      *
C         - the NS starting values, XSTART, of the  state variables which    *
C         are to be integrated from T1 to T2 with accuracy EPS, using the    *
```

```
C       NA algebraic  variables A. H1 should be set as a  guessed first      *
C       stepsize, HMIN as the minimum  allowed  stepsize. On output NOK       *
C       and NBAD are the numbers of good and bad (but retried and fixed)      *
C       steps taken, and XSTART is replaced by the values at the end of       *
C       the integration interval.                                             *
C       - DERIVS is the  user-supplied  subroutine for  calculating the       *
C       right-hand side derivative. (Bsstep is the name of the  stepper       *
C       routine to be used, which performs the integration, while Pass_       *
C       Discont uses a  fourth-order  Runge-Kutta  method to bypass any       *
C       discontinuities.)                                                     *
C       - the COMMON  block /PATH/ in the STORE subroutine contains the       *
C       information about the  minimum span, DTSAV, between  successive       *
C       values of the  independent variable, TP, at which  intermediate       *
C       values, XP and AP, are to be stored. KOUNT is the  total number       *
C       of the intermediate values that have been saved, with a maximum       *
C       value of KMAX. (See included file ODEINT.PAS)                         *
C                                                                             *
C       NB : When changing the number of state or algebraic  variables,       *
C       remember to change the value of NSTATE or NALGE in the included       *
C       parameter file ODEINT.PAS.                                            *
C       Similarly, when changing the length of integration or the mini-       *
C       mum recording span (DTSAV), change KMAX correspondingly.              *
C       After editing ODEINT.PAR, remember to recompile this program.         *
C                                                                             *
C ****************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
      PARAMETER (NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)

      DOUBLE PRECISION XSTART,XSCAL,X,DXDT,A
      DOUBLE PRECISION T,T1,T2,H,H1,HMIN,HDID,HNEXT,BIG
      DOUBLE PRECISION ZERO,TWO,TINY
      PARAMETER (ZERO = 0.0,TWO = 2.0,TINY = 1.0E-30)
      DIMENSION XSTART(NS),XSCAL(NSTAT),
      DIMENSION X(NSTAT),DXDT(NSTAT),A(NA)
      EXTERNAL BSSTEP,DERIVS
5     FORMAT ('1:Discontinuity between ',F11.4,' and ',F11.4,' !    ',
     &     '          ')

      BIG = D/EPS
      T = T1
      H = SIGN(H1,T2-T1)
      KEND = 0
      DO 10 I=1,NS
       X(I) = XSTART(I)
10    CONTINUE
20    CONTINUE
C                                                          start of main calculation loop
       IF (T .EQ. ZERO) CALL DERIVS(X,DXDT,NS,A,NA,T)
       DO 30 I=1,NSTAT
        XSCAL(I) = ABS(X(I)) + ABS(H*DXDT(I)) + TINY
C                                                        scaling factor to monitor accuracy
30     CONTINUE
C                                                                    store results
       CALL STORE(X,NS,A,NA,T,KEND)
C                                                    ensure that no step overshoots the end
       IF ((T+H-T2)*(T+H-T1) .GT. ZERO) H = T2 - T
       NDIS = 0
       IF (H .LE. ZERO) PAUSE 'h = zero in ODEINT'
       HDID = HMIN
       CALL BSSTEP(X,DXDT,NS,A,NA,T,H,HDID,HNEXT,EPS,BIG,XSCAL,
     & NDIS,DERIVS)
       IF (NDIS .EQ. 1) THEN
        WRITE (*,5) T, (T+H)
```

```
          CALL PASS_DISCONT(X,DXDT,NS,A,NA,T,H,HMIN,EPS,BIG,XSCAL,
     &  DERIVS)
          WRITE (*,5) (T-H),T
          DO 40 I=1,NSTAT
C                                                                    recalculate scaling factor
           XSCAL(I) = ABS(X(I)) + ABS(H*DXDT(I)) + TINY
40        CONTINUE
          IF (H*0.1 .GT. HMIN) THEN
           HNEXT = H*0.1
          ELSE
           HNEXT = HMIN
          ENDIF
          NDIS = 0
         ENDIF
         IF (HDID .EQ. H) THEN
          NOK = NOK + 1
         ELSE
          NBAD = NBAD + 1
         ENDIF
         IF ((T-T2)*(T2-T1) .GE. ZERO) THEN
C                                                                    check if end has been reached
          KEND = 1
          DO 50 I=1,NSTAT
           XSTART(I) = X(I)
50        CONTINUE
C                                                                    recalculate DXDT and A
          CALL DERIVS(X,DXDT,NS,A,NA,T)
C                                                                    and save results at end of step
          CALL STORE(X,NS,A,NA,T,KEND)
          H1 = HNEXT
          RETURN
C                                                                    exit integrator
         ENDIF
         H = HNEXT
C                                                    recalculate DXDT and A before going back for the next step
         CALL DERIVS(X,DXDT,NS,A,NA,T)
        GOTO 20
        END

C ***********************************************************************
C                                                                      *
        SUBROUTINE STORE(X,NS,A,NA,T,KEND)
C                                                                      *
C       The COMMON block /PATH/ contains the information about the     *
C       minimum span, DTSAV, between successive values of the indepen- *
C       dent variable, TP, at which intermediate values, XP, are to be stored. *
C       KOUNT is the total number of the intermediate values that have been *
C       saved, with a maximum value of KMAX.                           *
C                                                                      *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NCOMP = 18, NTOTS = 2,  KMAX  = 10)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)

        DOUBLE PRECISION X,A,T,TP,TSAV,XP,AP
        COMMON /UNICO/ MUNIT(NTYP1),LUNIT
        COMMON /PATH/ XP(NSTAT,KMAX),AP(NALGB,KMAX),TP(KMAX),
     & TSAV,DTSAV,KOUNT
        DIMENSION X(NS),A(NA)
15      FORMAT(F12.4,3X,F9.4,3X,F9.4,3X,F9.4,3X,F9.4,11X)

        IF ((KMAX .GT. 0) .AND. (KOUNT .LT. KMAX-1)) THEN
         IF ((KEND .EQ. 1) .OR. (ABS(T-TSAV) .GT. ABS(DTSAV))) THEN
C                                                    store only final or new intermediate results
```

```
            KOUNT = KOUNT + 1
            TP(KOUNT) = T
            TSAV = T
            DO 10 I=1,NSTAT
              XP(I,KOUNT) = X(I)
10          CONTINUE
            DO 20 I=1,NALGB
              AP(I,KOUNT) = A(I)
20          CONTINUE
           ENDIF
          ENDIF
c         WRITE (*,15) T,A(32),A(40),A(46),A(50)
          RETURN
          END

C *****************************************************************************
C                                                                               *
          SUBROUTINE BSSTEP(X,DXDT,NS,A,NA,T,HTRY,HDID,HNEXT,EPS,
     &BIG,XSCAL,NDIS,DERIVS)
C                                                                               *
C         Bulirsch-Stoer step with monitoring of local truncation error         *
C         to ensure accuracy and adjust stepsize. Input are the dependent       *
C         state variable vector X and its derivative DXDT, of length NS,        *
C         at the starting value of the independent variable T. Also input       *
C         the stepsize to be attempted HTRY, the required accuracy EPS,         *
C         and the vector XSCAL against which the error is scaled. On out-       *
C         put, X, A and T are replaced by the new values, HDID is the           *
C         stepsize which was actually accomplished and HNEXT is the esti-       *
C         mated next stepsize. DERIVS is the user-supplied subroutine           *
C         that computes the right-hand side derivatives.                        *
C                                                                               *
C         In the case where the error in any step is very large, and a          *
C         discontinuity is suspected, the flag NDIS is changed to 1. Then       *
C         the program returns to ODEINT,from where PASS_DISCONT                 *
C         is called to pass the discontinuity.                                  *
C                                                                               *
C         All 'print' statements are used in debugging and are thus optional.   *
C                                                                               *
C *****************************************************************************

          PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
          PARAMETER (NCOMP = 18, NTOTS = 2,  NUSE  = 6, IMAX = 6)
          PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                     + NCONN*2)
          PARAMETER (NSTAT = NUNIT*NCOMP)

          DOUBLE PRECISION X,XSCAL,XERR,X1,XSAV,DXDT,DXSAV,XSEQ,EXT,A
          DOUBLE PRECISION T,TSAV,H,HTRY,HDID,HNEXT,HMIN,TEST,TK
          DOUBLE PRECISION ERRMAX,BIG,BIGN
          DOUBLE PRECISION ZERO,ONE,TINY
          PARAMETER (SHRINK = 0.95,GROW = 1.2,TINY = 1.0E-30)
          PARAMETER (ZERO = 0.0, ONE = 1.0)
          COMMON /KEEP/ EXT(NSTAT,NUSE),TK(NSTAT)
          DIMENSION X(NS),DXDT(NS),XSCAL(NSTAT),XERR(NSTAT),
          DIMENSION X1(NSTAT),XSAV(NSTAT),DXSAV(NSTAT)
          DIMENSION XSEQ(NSTAT),NSEQ(IMAX),A(NA)
          EXTERNAL DERIVS
          DATA NSEQ /2,4,6,8,10,12/

          H=HTRY
          if (h .le. zero) pause 'stop 3 !'
          TSAV = T
          HMIN = HDID
c           print *,'TIME= ',T
          DO 10 I=1,NS
            XSAV(I) = X(I)
            DXSAV(I) = DXDT(I)
```

```
C                                                                keep the starting values
10    CONTINUE
20    CONTINUE
      EPSN = ABS(EPS/H**0.5)
      BIGN = ABS(BIG/H**0.5)
      DO 60 I=1,IMAX
C                                                  evaluate sequence of modified midpoint integrations
       CALL MMID(XSAV,DXSAV,XSEQ,NS,A,NA,TSAV,H,NSEQ(I),DERIVS)
       TEST = (H/NSEQ(I))**2.0
C                                                  this is squared because the error series is even
       CALL RZEXTR(XSEQ,X1,XERR,NS,TEST,I)
       ERRMAX = ZERO
       DO 30 J=1,NSTAT
        ERRMAX = MAX(ERRMAX,ABS(XERR(J)/XSCAL(J)))
30     CONTINUE
       if (errmax .gt. 1.0E+30) errmax=1.0E+30
       ERRMAX = ERRMAX/EPSN
       IF (ERRMAX .LT. ONE) THEN
C                                                  a) this step has been successfully integrated
        DO 40 J=1,NSTAT
         X(J) = X1(J)
40      CONTINUE
        T = T + H
        HDID = H
        IF (I .EQ. NUSE-2) THEN
         HNEXT = H*SHRINK
        ELSE IF (I .EQ. NUSE-3) THEN
         HNEXT = H*GROW
        ELSE
         IF (H .GE. ONE) THEN
          HNEXT = H*(NSEQ(NUSE-1)*1.0)/(NSEQ(I)*1.0)
         ELSE
C                                                  ensure that step won't grow too fast after discontinuity
          HNEXT = H*(1.0 + (NSEQ(NUSE-3)*1.0)/(NSEQ(I)*1.0))/2.0
         ENDIF
        ENDIF
        IF (HNEXT .LT. HMIN) HNEXT = HMIN
        RETURN
       ELSEIF (ERRMAX .GT. BIGN) THEN
        IF (NDIS .EQ. 0) THEN
C                                                  b) use alternative method as this step contains a dis.
         NDIS = 1
         HDID = ZERO
         DO 50 J=1,NSTAT
          DXDT(J) = DXSAV(J)
          X(J) = XSAV(J)
50       CONTINUE
         RETURN
        ELSE
C                                                  unless dis. has already been discovered
        ENDIF
       ENDIF
60    CONTINUE
      IF (H .LE. HMIN) THEN
C                                                  we have to accept the error
       DO 70 J=1,NSTAT
        X(J) = X1(J)
70     CONTINUE
       T = T + H
       HDID = H
       HNEXT = H
       RETURN
      ENDIF
      H = 0.25*H
C                                                  c) try using a smaller step as error is too large
      IF (H .LT. HMIN) THEN
       H = HMIN
```

```
      ENDIF
      GOTO 20
      END

C ***********************************************************************
C                                                                       *
      SUBROUTINE MMID(X,DXDT,XOUT,NS,A,NA,TS,HTOT,NSTEP,DERIVS)
C                                                                       *
C     Modified midpoint step. Dependent variable vector X of length     *
C     NS and its derivative vector DXDT are input at TS. Also input     *
C     is HTOT, the total step to be made, and NSTEP, the number of      *
C     substeps to be used. The output is returned as XOUT, which need   *
C     not be a distinct array from X; if it is different, however,      *
C     then X and DXDT are returned undamaged.                           *
C                                                                       *
C ***********************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
      PARAMETER (NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)

      DOUBLE PRECISION X,DXDT,XOUT,XM,XN,SWAP,A,ZERO
      DOUBLE PRECISION T,TS,H,HTOT
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),DXDT(NS),XOUT(NS),XM(NSTAT),
     &     XN(NSTAT),A(NA)
      EXTERNAL DERIVS
      H = HTOT/NSTEP
C                                                   find stepsize for this round
      DO 10 I=1,NSTAT
        XM(I) = X(I)
        XN(I) = X(I) + H*DXDT(I)
        XOUT(I) = ZERO
C                                                                  first step
10    CONTINUE
      T = TS + H
      CALL DERIVS(XN,XOUT,NS,A,NA,T)
C                                          use XOUT for temp. storage of derivatives
      H2 = 2.0*H
      DO 30 N=2,NSTEP
        DO 20 I=1,NSTAT
          SWAP = XM(I) + H2*XOUT(I)
          XM(I) = XN(I)
          XN(I) = SWAP
C                                                                  general step
20      CONTINUE
        T = T + H
        CALL DERIVS(XN,XOUT,NS,A,NA,T)
30    CONTINUE
      DO 40 I=1,NSTAT
        XOUT(I) = 0.5*(XM(I) + XN(I) + H*XOUT(I))
C                                                                  last step
40    CONTINUE
      RETURN
      END

C ***********************************************************************
C                                                                       *
      SUBROUTINE RZEXTR(XEST,XZ,DX,NS,TEST,IEST)
C                                                                       *
C     Use diagonal rational function extrapolation to evaluate NS       *
C     functions at T=0 by fitting a diagonal rational function to a     *
C     sequence of estimates with progressively smaller values T=TEST,   *
C     and corresponding function vectors XEST. This call is number      *
C     IEST in the sequence of calls. The extrapolation uses only the    *
```

```
C       last NUSE estimates. Extrapolated function values are output as      *
C       XZ, and their estimated error is output as DX.                       *
C                                                                            *
C ***************************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
        PARAMETER (NCOMP = 18, NTOTS = 2,  NUSE = 6)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)

        DOUBLE PRECISION XEST,XZ,DX,EXT,FT,XX,V,C,B1,B,DDX,TEST,TK
        DOUBLE PRECISION ZERO
        DIMENSION XEST(NS),XZ(NS),DX(NS),FT(NUSE)
        PARAMETER (ZERO = 0.0)
        COMMON /KEEP/ EXT(NSTAT,NUSE),TK(NSTAT)

        TK(IEST) = TEST
C                                                   keep the current value of independent variable
        IF (IEST .EQ. 1) THEN
          DO 10 J=1, NSTAT
            XZ(J) = XEST(J)
            EXT(J,1) = XEST(J)
            DX(J) = XEST(J)
10        CONTINUE
        ELSE
          M1 = MIN(IEST,NUSE)
C                                                   use at most NUSE previous values
          DO 20 K=1, M1-1
            FT(K+1) = TK(IEST-K)/TK(IEST)
20        CONTINUE
          DO 40 J=1,NSTAT
C                                                   evaluate next diagonal in tableau
            XX = XEST(J)
            V = EXT(J,1)
            C = XX
            EXT(J,1) = XX
            DO 30 K=2,M1
              B1 = FT(K)*V
              B = B1 - C
              IF (B .NE. ZERO) THEN
                B = (C-V)/B
                DDX = C*B
                C = B1*B
              ELSE
                DDX = V
C                                                   so that we don't divide by 0 later
              END IF
              IF (K .NE. M1) V = EXT(J,K)
              EXT(J,K) = DDX
              XX = XX + DDX
30          CONTINUE
            DX(J) = DDX
            XZ(J) = XX
40        CONTINUE
        END IF
        RETURN
        END

C ***************************************************************************
C                                                                            *
        SUBROUTINE PASS_DISCONT(XO,DXDT,NS,A,NA,T1,H,HMIN,EPS,
     &BIG,XSCAL,DERIVS)
C                                                                            *
C       This procedure finds the order and location of a discontinuity       *
C       (dis.) according to the method proposed by Gear & Osterby:           *
C       Each step is tested for the presence of the dis. by  comparing       *
```

```
C       the results of each integration step with the  result obtained      *
C       by doing two half-steps. If the error is larger  than BIG, the      *
C       dis. is  assumed to lie within  the step, and the  integration       *
C       therefore  fails. Depending on the  sequence of  successes and       *
C       failures, and  using the  calculated  slopes, the order can be       *
C       determined.                                                          *
C       Once the location can be determined exactly or the integration       *
C       step is small enough to limit the error,the method steps right       *
C       up to or just over the dis. and then restarts.                       *
C                                                                            *
C ***************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
      PARAMETER (NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION XO,DXDT,XSCAL,XF,XM,XF2,DXMDT,A
      DOUBLE PRECISION ERRMAX,T1,T2,TM,TEND,H,HMIN,HPASS,HREM
      DOUBLE PRECISION ALPHA,AK1,AK2,AK3,D1,D2,D1NEW,D2NEW
      DOUBLE PRECISION XMMAX,ZERO,TWO,TINY,BIG,BIGN
      PARAMETER (SAFETY = 0.9, PSHRINK = -0.25, TINY = 1.0E-30)
      PARAMETER (ZERO = 0.0, TWO = 2.0)
      DIMENSION XO(NS),DXDT(NS),XSCAL(NS),XF(NSTAT),XM(NSTAT)
      DIMENSION XF2(NSTAT),DXMDT(NSTAT),A(NA)
      EXTERNAL DERIVS,RK4,BSSTEP
5     FORMAT ('2:Discontinuity between ',F13.6,' and ',F13.6,' ! ',
     &     '          ')

      NORDER = 1
      NCONFIRM = 0
      NFAIL = 0
      NSUCCESS = 0
      ALPHA = ZERO
      D1NEW = ZERO
      D2NEW = ZERO
      D2 = ZERO
      DO 10 J=1,NSTAT
       XF(J) = ZERO
       XF2(J) = ZERO
       XM(J) = ZERO
       DXMDT(J) = ZERO
10    CONTINUE

      TEND = T1+H
      H = H/TWO
C                                                          test 1st half step
      CALL RK4(XO,DXDT,XF,NS,A,NA,T1,H,DERIVS)
C                                          initially assume 1st order and calculate D1
      AK1 = ZERO
      NORDER = 1
      DO 20 I=1,NSTAT
       AK1 = MAX(AK1,ABS(XF(I) - XO(I)))
20    CONTINUE
      D1 = AK1/H
      HPASS = EPS/AK1
C                                                          Start of main loop:
30    CONTINUE
       IF ((TEND-T1) .LE. ZERO) THEN
C                                                  end of interval was reached
        T1 = TEND
        CALL DERIVS(XO,DXDT,NS,A,NA,T1)
        RETURN
       ENDIF
       IF (H .LT. TWO*HMIN) THEN
```

```
C                                                                    this will be last step
      H = TWO*HMIN
      CALL RK4(XO,DXDT,XF,NS,A,NA,T1,H,DERIVS)
      ENDIF
      WRITE (*,5) T1, (T1 + 2.0*H)
      EPSN = ABS(EPS/H**0.5)
      BIGN = ABS(BIG/H**0.5)
C                                                  1) Calculate error when step length is halved
      H = H/TWO
      NSTEP = 3
      CALL MMID(XO,DXDT,XM,NS,A,NA,T1,H,NSTEP,DERIVS)
c      print *,'    TESTING BETWEEN',T1,' AND',T1+2*H
      TM = T1 + H
      CALL DERIVS(XM,DXMDT,NS,A,NA,TM)
      CALL MMID(XM,DXMDT,XF2,NS,A,NA,TM,H,NSTEP,DERIVS)

      ERRMAX = ZERO
      DO 40 I=1,NSTAT
       ERRMAX = MAX(ERRMAX,ABS((XF2(I) - XF(I))/XSCAL(I)))
40    CONTINUE
      IF (ERRMAX .GT. 1.0E+30) ERRMAX = 1.0E+30
      ERRMAX = ERRMAX/EPSN
C                                                  2) Find order and location of dis.
      IF (ERRMAX .GT. BIGN) THEN
C                                                        dis. lies in the 1st half step
       AK1 = ZERO
       DO 50 I=1,NSTAT
        AK1 = MAX(AK1,ABS(XM(I) - XO(I)))
50     CONTINUE
       D1NEW = AK1/H

       IF (D2 .EQ. ZERO) THEN
C                                                  we have previous info on D1 only
        IF (D1NEW .GT. D1) THEN
C                                                  either the dis. is 1st order
         NORDER = 1
         NCONFIRM = NCONFIRM + 1
         HPASS = EPS/AK1
        ELSE
C                                                  or the dis. is 2nd order
         AK2 = ZERO
         DO 60 I=1,NSTAT
          AK2 = MAX(AK2,ABS(XF2(I) - TWO*XM(I) + XO(I)))
60       CONTINUE
         D2NEW = AK2/(TWO*H*H)
         NORDER = 2
         NCONFIRM = 0
        ENDIF
       ELSE
C                                                  we have previous info on both D1 and D2
        AK1 = ZERO
        DO 70 I=1,NSTAT
         AK1 = MAX(AK1,ABS(XF2(I) - XO(I)))
70      CONTINUE
        D1NEW = AK1/H

        IF (D1NEW .GT. D1) THEN
         IF (NORDER .NE. 1) THEN
          NORDER = 1
          NCONFIRM = 0
         ELSE
          NCONFIRM = NCONFIRM + 1
         END IF
         HPASS = EPS/AK1
        ELSE
         AK2 = ZERO
         DO 80 I=1,NSTAT
```

```
            AK2 = MAX(AK2,ABS(XF2(I) - TWO*XM(I) + XO(I)))
80          CONTINUE
            D2NEW = AK2/(TWO*H*H)

            IF (NFAIL .GE. 2) THEN
C                                                   at least two successive steps contained the dis.
             IF (D2NEW .GT. TWO*D2) THEN
              IF (NORDER .EQ. 2) THEN
               NCONFIRM = NCONFIRM + 1
              ELSE
               NORDER = 2
               NCONFIRM = 0
              ENDIF
              AK2 = ZERO
              XMMAX = ZERO
              DO 90 I=1,NSTAT
               AK2 = MAX(AK2,ABS(XF2(I) - XM(I)))
               XMMAX = MAX(XMMAX,(XM(I) - XO(I)))
90            CONTINUE
              AK2 = AK2/H
              HPASS = SQRT(EPS/AK2)
              ALPHA = TM-XMMAX/AK2
             ELSE
              IF (NORDER .EQ. 3) THEN
               NCONFIRM = NCONFIRM+1
              ELSE
               NORDER = 3
               NCONFIRM = 0
              ENDIF
              AK3 = TWO*D2NEW
              HPASS = (TWO*EPS/AK3)**(1.0/3.0)
             ENDIF
            ELSE
C                                                   previous step didn't contain dis., but this one does
             IF (D2NEW .GT. TWO*D2) THEN
              IF (NORDER .EQ. 2) THEN
               NCONFIRM = NCONFIRM + 1
              ELSE
               NORDER = 2
               NCONFIRM = 0
              ENDIF
              AK2 = ZERO
              XMMAX = ZERO
              DO 100 I=1,NSTAT
               AK2 = MAX(AK2,ABS(XF2(I) - XM(I)))
               XMMAX = MAX(XMMAX,(XM(I) - XO(I)))
100           CONTINUE
              AK2 = AK2/H
              HPASS = SQRT(EPS/AK2)
              ALPHA = TM-XMMAX/AK2
             ELSE
             ENDIF
            ENDIF
           ENDIF
          ENDIF
          D2 = D2NEW
          D1 = D1NEW
          NFAIL = NFAIL + 1
         ELSE
          IF (ERRMAX .GT. 1.0) THEN
C                                                   the accuracy of integration is not satisfactory
           DO 110 I=1,NSTAT
            XM(I) = XO(I)
110        CONTINUE
C                                                   therefore calculate new XM
           TM = T1 + H
           HREM = H
```

```
            CALL DRIVER2(XM,DXDT,NS,A,NA,T1,TM,H,HMIN,EPS,BIG,
     &           XSCAL,DERIVS,BSSTEP)
            CALL DERIVS(XM,DXMDT,NS,A,NA,TM)
            DO 120 I=1,NSTAT
              XF2(I) = XM(I)
120         CONTINUE
C                                                                  and new XF2
            H = HREM
            T2 = TM + H
            CALL DRIVER2(XF2,DXMDT,NS,A,NA,TM,T2,H,HMIN,EPS,BIG,
     &           XSCAL,DERIVS,BSSTEP)
            H = HREM
           ENDIF
C                                                                  dis. lies in 2nd half step
           IF (NFAIL .GE. 1) THEN
C                                                                  deduction possible as previous step failed
            AK2 = ZERO
            DO 130 I=1,NSTAT
              AK2 = MAX(AK2,ABS(XF2(I) - TWO*XM(I) + XO(I)))
130         CONTINUE
            D2NEW = AK2/(TWO*H*H)

            IF (D2NEW .GE. 0.65*D2) THEN
              IF (NORDER .EQ. 2) THEN
                NCONFIRM = NCONFIRM + 1
              ELSE
                NORDER = 2
                NCONFIRM = 0
              ENDIF
            ELSE
            ENDIF
            D1 = D1NEW
            D2 = D2NEW
           ELSE
C                                                                  no deduction possible
            ENDIF
            NFAIL = 0
          ENDIF
          IF (HPASS .LT. (1.1*HMIN)) HPASS = 1.1*HMIN

C                                                                  3) Decide whether to restart or to take more steps
          IF (H .GT. HPASS) THEN
            IF (NFAIL .EQ. 0) THEN
              T1 = T1 + TWO*H
C                                                                  step forward to the endpt for another step
              DO 140 I=1,NSTAT
                XO(I) = XF2(I)
140           CONTINUE
              CALL DERIVS(XO,DXDT,NS,A,NA,T1)
              CALL RK4(XO,DXDT,XF,NS,A,NA,T1,H,DERIVS)
            ELSE
C                                                                  take another step from original start
              DO 150 I=1,NSTAT
                XF(I) = XM(I)
150           CONTINUE
            END IF
            GOTO 30
          ELSE
            H = TWO*H
            IF (NFAIL .EQ. 0) THEN
              IF (NSUCCESS .EQ.1) THEN
C                                                                  if 2 equal successive steps were successful, restart
                T1 = T1+H
                DO 160 I=1,NSTAT
                  XO(I) = XF2(I)
160             CONTINUE
                RETURN
```

```
            ELSE
             IF ((NORDER .EQ. 2) .AND. (NCONFIRM .NE. 0)) THEN
C                                                          restart ONLY if dis. is definitely 2nd order
              IF ((ALPHA .GT. (T1+H)) .AND. (ALPHA .LT.(T1+2*H))) THEN
C                                                          AND if alpha lies within the next step
               KEND = 1
               CALL STORE(XF2,NS,A,NA,T1,KEND)
               T1 = T1+H
               H = (ALPHA-T1)*1.05
C                                                          go just beyond the dis.
               CALL DERIVS(XF2,DXDT,NS,A,NA,T1)
               CALL RK4(XF2,DXDT,XO,NS,A,NA,T1,H,DERIVS)
               T1 = T1 + H
               RETURN
              ENDIF
             ENDIF

C                                          otherwise take another step equal to one before from prev endpoint
             T1 = T1 + H
             DO 170 I=1,NSTAT
              XO(I) = XF2(I)
170          CONTINUE
             KEND = 1
             CALL STORE(XO,NS,A,NA,T1,KEND)
             CALL DERIVS(XO,DXDT,NS,A,NA,T1)
             CALL RK4(XO,DXDT,XF,NS,A,NA,T1,H,DERIVS)
             NSUCCESS = 1
             GOTO 30
            ENDIF
           ELSE
C                                                  dis. overstepped in small enough step, therefore restart
            T1 = T1 + H
            DO 180 I=1,NSTAT
             XO(I) = XF2(I)
180         CONTINUE
            RETURN
           ENDIF
          ENDIF
         END

C ***********************************************************************
C                                                                       *
         SUBROUTINE RK4(X,DXDT,XOUT,NS,A,NA,T,H,DERIVS)
C                                                                       *
C        Given values for NS variables X and their derivatives DXDT,    *
C        known at T, use the 4th-order Runge-Kutta method to advance the *
C        solution over an interval H and return the incremented varia-  *
C        bles as XOUT, which need not be distinct from X. The user sup- *
C        plies the subroutine DERIVS which returns DXDT and A at T.     *
C                                                                       *
C ***********************************************************************

         PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
         PARAMETER (NCOMP = 18, NTOTS = 2)
         PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                    + NCONN*2)
         PARAMETER (NSTAT = NUNIT*NCOMP)

         DOUBLE PRECISION X,DXDT,XOUT,XT,DXT,DXM,A,T,TH,H,HH,H6
         DOUBLE PRECISION ZERO
         PARAMETER (ZERO = 0.0)
         DIMENSION X(NS),DXDT(NS),XOUT(NS),XT(NSTAT),DXT(NSTAT),
     & DXM(NSTAT),A(NA)
         EXTERNAL DERIVS

         HH = H*0.5
         H6 = H/6.0
```

```
      TH = T + HH
      DO 10 I=1,NSTAT
C                                                                    first step
        DXT(I) = ZERO
        DXM(I) = ZERO
        XT(I) = X(I) + HH*DXDT(I)
10    CONTINUE
      CALL DERIVS(XT,DXT,NS,A,NA,TH)
C                                                                    second step
      DO 20 I=1,NSTAT
        XT(I) = X(I) + HH*DXT(I)
20    CONTINUE
      CALL DERIVS(XT,DXM,NS,A,NA,TH)
C                                                                    third step
      DO 30 I=1,NSTAT
        XT(I) = X(I) + H*DXM(I)
        DXM(I) = DXT(I) + DXM(I)
30    CONTINUE
      CALL DERIVS(XT,DXT,NS,A,NA,T+H)
C                                                                    fourth step
      DO 40 I=1,NSTAT
        XOUT(I) = X(I) + H6*(DXDT(I) + DXT(I) + 2.*DXM(I))
C                                                                    accumulate increments with proper weights
40    CONTINUE
      RETURN
      END

C ***********************************************************************
C                                                                      *
      SUBROUTINE DRIVER2(XSTART,DXDT,NS,A,NA,T1,T2,H1,HMIN,EPS,BIG,
     *XSCAL,DERIVS,BSSTEP)
C                                                                      *
C     This driver is similar to the ODEINT  subroutine, but is called  *
C     only from the PASS_DISCONT routine when more  accurate integra-  *
C     tion of discontinuity-free steps is needed.                      *
C                                                                      *
C ***********************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40)
      PARAMETER (NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                 + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)

      DOUBLE PRECISION XSTART,XSCAL,DXDT,X,A
      DOUBLE PRECISION T,T1,T2,H,H1,HMIN,HNEXT,HDID,BIG
      DOUBLE PRECISION ZERO,TWO,TINY
      PARAMETER (ZERO = 0.0, TWO = 2.0, TINY = 1.E-30)
      DIMENSION XSTART(NS),XSCAL(NS),DXDT(NS),X(NSTAT),A(NA)
      EXTERNAL DERIVS,BSSTEP,STORE

      T = T1
      KEND = 0
      H = SIGN(H1,T2-T1)
c      print *,'H=',H
      DO 10 I=1,NSTAT
        X(I) = XSTART(I)
10    CONTINUE
20    CONTINUE
        CALL STORE(X,NS,A,NA,T,KEND)
        NDIS = 1
        HDID = HMIN
        IF ((T+H-T2)*(T+H-T1) .GT. ZERO) H = T2 - T
        if (H .le. ZERO) pause 'stop 2 !'
        CALL BSSTEP(X,DXDT,NS,A,NA,T,H,HDID,HNEXT,EPS,BIG,XSCAL,
     &            NDIS,DERIVS)
        IF (ABS(T-T2) .NE. ZERO) THEN
```

```
            CALL DERIVS(X,DXDT,NS,A,NA,T)
           ENDIF
           IF ((T-T2)*(T2-T1) .GE. ZERO) THEN
            KEND = 1
            DO 30 I=1,NSTAT
             XSTART(I) = X(I)
30          CONTINUE
            CALL STORE(X,NS,A,NA,T,KEND)
            H1 = HNEXT
            RETURN
           ENDIF
           H = HNEXT
          GOTO 20
          END

C ***************************************************************************
C                                                                           *
C    Copyright (c) MINTEK 1992. Right of Reproduction Reserved.             *
C                                                                           *
C ***************************************************************************
```

I.3 DERIV.F : DERIVATIVES SUBROUTINE

```
C         This file contains the master derivative  subroutine and  those   *
C         subroutines which calculate the actual derivatives of the state   *
C         variables.                                                        *
C                                                                           *
C ***************************************************************************
C                                                                           *
          SUBROUTINE DERIVS(X,DX,NS,A,NA,T)
C                                                                           *
C         The differentiation procedure returns the values of the deriva-   *
C         tives DX at time T, which it calculates using the values of the   *
C         state variables X at T. All algebraic variables A are first cal-  *
C         culated, before DX can be evaluated. This particular subroutine   *
C         selects the  applicable  subroutine to  calculate the algebraic   *
C         variables of each unit, stream or connection. Only after it has   *
C         checked that all algebraic variables have been  calculated does   *
C         it then select the particular unit-routine to calculate the de-   *
C         rivatives of the state variables for the unit being considered.   *
C                                                                           *
C         The types of units are:                                           *
C          1 : feed unit                2 : sink unit                     *
C          3 : mixer                    4 : screen                        *
C          5 : tank                     6 : leach pachuca                 *
C          7 : CIP tank                 8 : component changer             *
C                                                                           *
C ***************************************************************************

          PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
          PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
          PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                     + NCONN*2)
          PARAMETER (NSTAT = NUNIT*NCOMP)
          PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

          DOUBLE PRECISION X,DX,A,T,ZERO,CONV,TRLIMIT,CCLIMIT
          INTEGER UNIT, STREAM, CONN
          PARAMETER (ZERO = 0.0, PI = 3.1415927)
          DIMENSION X(NS),DX(NS),A(NA)

          COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
          COMMON /ALALG/ KALG(NPROC)
          COMMON /MNNDV/ KALLS,kalls2,KROUND
          COMMON /UNICO/ MUNIT(NTYP1),LUNIT
```

```
      COMMON /SCREN/ NOONE
      COMMON /FEEDS/ OPTSIM,DAT(18),LUAT
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /CARBN/ FLO(NSTRM),HLA(NUNIT),HLD(NUNIT),NCOND2
5     FORMAT (F12.4,51X,I2,I6)

      KREP = 0
      LUNIT = 0
      NOONE = 1
      DO 10 I=1,NPROC
       KALG(I) = 0
10    CONTINUE
      DO 20 J=1,NS
       DX(J) = ZERO
20    CONTINUE
      TRLIMIT = 5000.0/PHYS(2,7,1)
      CCLIMIT = 0.02*PI*3.5*3.5*5.3/CONV(2,7)

30    CONTINUE
C                                                    initially calculate all algebraic variables
      DO 40 L=1,NUNIT
       IF (KALG(L) .EQ. 0) THEN
        LU1 = UNIT(L,1)
        IF   (LU1 .EQ. 1) THEN
C                                                    calculate algebraic variables of feed units the first time only
         IF (KROUND .EQ. 0) THEN
          CALL ALGU(X,NS,A,NA,T,L)
         ELSE
          KALG(L) = 1
         ENDIF
C                                                    calculate algebraic variables for only those units with hold up
        ELSEIF ((LU1 .EQ. 2) .OR. (LU1 .EQ. 5) .OR. (LU1 .EQ. 6) .OR.
     &  (LU1 .EQ. 7)) THEN
         CALL ALGU(X,NS,A,NA,T,L)
        ELSE
C                                                    for the other units, alg vars remain zero
         KALG(L) = 1
        ENDIF
       ENDIF
40    CONTINUE
      DO 80 I=1,NSTRM
       IF (KALG(NUNIT+I) .EQ. 0) THEN
        IF (STREAM(I,1) .EQ. 0) THEN
C                                                    for non-connected streams, set KALG = 1
         KALG(NUNIT+I) = 1
        ELSE
         DO 70 L=1,NUNIT
          IF (STREAM(I,1) .EQ. L) THEN
           IF    (UNIT(L,1) .EQ. 1) THEN
            IF (OPTSIM .EQ. '3') THEN
             CALL ALGS1(X,NS,A,NA,T,I,L)
            ELSE
             CALL ALGS1(X,NS,A,NA,T,I,L)
            ENDIF
           ELSEIF (UNIT(L,1) .EQ. 2) THEN
            KALG(NUNIT+I) = 1
           ELSEIF (UNIT(L,1) .EQ. 3) THEN
            CALL ALGS3(X,NS,A,NA,T,I,L)
           ELSEIF (UNIT(L,1) .EQ. 4) THEN
            CALL ALGS4(X,NS,A,NA,T,I,L)
           ELSEIF (UNIT(L,1) .EQ. 5) THEN
            IF (X(INX(L)+1).GT.ZERO) THEN
             CALL ALGS5(X,NS,A,NA,T,I,L)
            ELSE
             KALG(NUNIT+I) = 1
             DO 50 J=1,(NCOMP+NTOTS)
              A(INA(NUNIT+I)+J) = ZERO
```

```
50              CONTINUE
               ENDIF
              ELSEIF (UNIT(L,1) .EQ. 6) THEN
               IF (X(INX(L)+1).GT.ZERO) THEN
                CALL ALGS6(X,NS,A,NA,T,I,L)
               ELSE
                KALG(NUNIT+I) = 1
                DO 60 J=1,(NCOMP+NTOTS)
                 A(INA(NUNIT+I)+J) = ZERO
60              CONTINUE
               ENDIF
              ELSEIF (UNIT(L,1) .EQ. 7) THEN
               CALL ALGS7(X,NS,A,NA,T,I,L)
              ELSEIF (UNIT(L,1) .EQ. 8) THEN
               CALL ALGS8(X,NS,A,NA,T,I,L)
              ENDIF
             ENDIF
70          CONTINUE
           ENDIF
          ENDIF
80      CONTINUE
        DO 90 I=1,NCONN
         IF (KALG(NUNIT+NSTRM+I) .EQ. 0 ) THEN
          KALG(NUNIT+NSTRM+I) = 1
         ENDIF
90      CONTINUE

        KALL = 1
        DO 100 I=1,NPROC
C                                                   if any algebraic variables have not been calculated
         IF (KALG(I) .EQ. 0) THEN
          PRINT *,I,'KALG=',KALG(I)
          KALL = 0
         ENDIF
100     CONTINUE
C                                                                   go back to calculate them
        IF (KALL .EQ. 0) THEN
         IF (KREP .LE. 3) THEN
          KREP = KREP + 1
          GOTO 30
         ELSE
          PRINT *,'Problem with calculation of algebraic variables !'
          STOP
         ENDIF
        ENDIF
C                                                   otherwise continue by calculating the derivatives
        DO 120 L=1,NUNIT
         LU1 = UNIT(L,I)
         IF (LU1 .EQ. 1) THEN
          DO 110 J=1,NCOMP
           DX(INX(L)+J) = ZERO
C                                                   state variables in feed units don't change
110       CONTINUE
         ELSEIF (LU1 .EQ. 2) THEN
          CALL DIF2(X,DX,NS,A,NA,T,L)
         ELSEIF (LU1 .EQ. 5) THEN
          CALL DIF5(X,DX,NS,A,NA,T,L)
         ELSEIF (LU1 .EQ. 6) THEN
          CALL DIF6(X,DX,NS,A,NA,T,L)
         ELSEIF (LU1 .EQ. 7) THEN
          CALL DIF7(X,DX,NS,A,NA,T,L)
         ENDIF
120     CONTINUE
        KALLS = KALLS + 1
        KROUND = 1
        IF (KALLS .EQ. 10000) THEN
         KALLS = 0
```

```
          KALLS2 = KALLS2 + 1
        ENDIF
        RETURN
        END

C ***********************************************************************
C                                                                       *
      SUBROUTINE DIF2(X,DX,NS,A,NA,T,L)
C                                                                       *
C     This is the subroutine to calculate the derivatives of the        *
C     state variables associated with a sink unit.                      *
C                                                                       *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NTYP2 = 2, NCOMP = 18, NTOTS = 2, NREAC = 12)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)
        PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

        DOUBLE PRECISION X,DX,A,T,ZERO,CONV,RATE,XR
        INTEGER UNIT, STREAM, CONN
        PARAMETER (ZERO = 0.0)
        DIMENSION X(NS),DX(NS),A(NA),XR(NCOMP),XE(NCOMP)
        DIMENSION RATE(NREAC)

        COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
        COMMON /CARBN/ FLO(NSTRM),HLA(NUNIT),HLD(NUNIT),NCOND2

        TA = T
        LU1 = UNIT(L,1)
        LU2 = UNIT(L,2)
C                                                   calculate differentials of tank components
        DO 20 J=1,NCOMP
          DX(INX(L)+J) = ZERO
          DO 10 I=1,NSTRM
C                                                   add mols from any incoming stream
            IF (STREAM(I,2) .EQ. L) DX(INX(L)+J) = DX(INX(L)+J) +
     &                              A(INA(NUNIT+I)+J)
10        CONTINUE
20      CONTINUE
        RETURN
        END

C ***********************************************************************
C                                                                       *
      SUBROUTINE DIF5(X,DX,NS,A,NA,T,L)
C                                                                       *
C     This is the subroutine to calculate the derivatives of the        *
C     state variables associated with a tank.                           *
C                                                                       *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NTYP2 = 2, NCOMP = 18, NTOTS = 2, NREAC = 12)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)
        PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

        DOUBLE PRECISION X,DX,A,T,ZERO,CONV,RATE,XR
        INTEGER UNIT, STREAM, CONN
        PARAMETER (ZERO = 0.0)
        DIMENSION X(NS),DX(NS),A(NA),XR(NCOMP),XE(NCOMP)
        DIMENSION RATE(NREAC)
```

```
      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /DIRIV/ STOI(NTYP2,NCOMP,NREAC),RK(NTYP2,NREAC)

      TA = T
      LU1 = UNIT(L,1)
      LU2 = UNIT(L,2)
      DO 10 J=1,NCOMP
       XE(J) = ZERO
10    CONTINUE
      XE(7) = 0.331E-06
      DO 20 K=1,NREAC
       RATE(K) = ZERO
20    CONTINUE

      IF (X(INX(L)+1) .GT. ZERO) THEN
       DO 30 J=1,NCOMP
C                                                  calculate concentrations in terms of liquid volumes (in kmol/l)
        XR(J) = X(INX(L)+J)/(X(INX(L)+1)*CONV(LU2,1)*1000.0)
30     CONTINUE
C                                                        calculate rates of the chemical reactions :
C                                                           if Ca(OH)2 is present, it dissociates
       IF (XR(3) .GE. 3.0E-9)
     &  RATE(1) = RK(LU2,1)*XR(3)*(1-XR(4)*XR(5)*XR(5)/2.937E-05)
C                                                  O2 dissolves in water if [O2] < its equilibrium value
       IF (XR(7) .LE. XE(7)) RATE(2) = RK(LU2,2)*(XE(7)-XR(7))
C                                                        only if O2 and CN- are present
       IF ((XR(7) .GT. ZERO) .AND. (XR(6) .GT. ZERO)) THEN
C                                                           CN- is oxydised to cyanate
        RATE(3) = RK(LU2,3)*XR(6)*XR(7)/XE(7)
C                                                           gold is dissolved
        RATE(4) = RK(LU2,4)*XR(8)/(6.316/XR(6) + 1/XR(7))
        RATE(5) = RK(LU2,5)*XR(9)/(6.316/XR(6) + 1/XR(7))
C                                                           metal is dissolved
        RATE(6) = RK(LU2,6)*XR(11)/(9.81/XR(6) + 1/XR(7))
        RATE(7) = RK(LU2,7)*XR(12)/(9.81/XR(6) + 1/XR(7))
       ENDIF
      ENDIF
C                                                        calculate differentials of tank components
      DO 60 J=1,NCOMP
       DX(INX(L)+J) = ZERO
       DO 40 I=1,NSTRM
C                                                           add mols from any incoming stream
        IF (STREAM(I,2) .EQ. L) DX(INX(L)+J) = DX(INX(L)+J) +
     &                          A(INA(NUNIT+I)+J)
C                                                           subtract mols for any leaving stream
        IF (STREAM(I,1) .EQ. L) DX(INX(L)+J) = DX(INX(L)+J) -
     &                          A(INA(NUNIT+I)+J)
40     CONTINUE
       IF (X(INX(L)+1) .GT. ZERO) THEN
        DO 50 K=1,NREAC
C                                        rates are in terms of concentrations, thus multiply by liquid volume
         DX(INX(L)+J) = DX(INX(L)+J) + STOI(LU2,J,K)*RATE(K)*
     &          X(INX(L)+1)*CONV(LU2,1)*1000.0
50      CONTINUE
       ENDIF
60    CONTINUE

      RETURN
      END

C ***************************************************************************
C                                                                            *
      SUBROUTINE DIF6(X,DX,NS,A,NA,T,L)
C                                                                            *
C     This is the subroutine to calculate the derivatives of the state       *
```

```
C       variables associated with leach pachuca L.                      *
C                                                                       *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NTYP2 = 2, NCOMP = 18, NTOTS = 2, NREAC = 12)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)
        PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

        DOUBLE PRECISION X,DX,A,T,ZERO,CONV,RATE,XR
        PARAMETER (ZERO = 0.0)
        INTEGER UNIT, STREAM, CONN
        DIMENSION X(NS),DX(NS),A(NA),XR(NCOMP),XE(NCOMP)
        DIMENSION RATE(NREAC)

        COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
        COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
        COMMON /DIRIV/ STOI(NTYP2,NCOMP,NREAC),RK(NTYP2,NREAC)

        TA = T
        LU1 = UNIT(L,1)
        LU2 = UNIT(L,2)
        DO 10 J=1,NCOMP
          XE(J) = ZERO
10      CONTINUE
        XE(7) = 0.331E-06
        DO 20 K=1,NREAC
          RATE(K) = ZERO
20      CONTINUE

        IF (X(INX(L)+1) .GT. ZERO) THEN
          DO 30 J=1,NCOMP
C                                                 calculate concentrations in terms of liquid volumes (in kmol/l)
            XR(J) = X(INX(L)+J)/(X(INX(L)+1)*CONV(LU2,1)*1000.0)
30        CONTINUE
C                                                       calculate rates of chemical reactions
C                                                       if Ca(OH)2 is present, it dissociates
          IF (XR(3) .GE. zero)
     &    RATE(1) = RK(LU2,1)*XR(3)*(1-XR(4)*XR(5)*XR(5)/2.937E-05)
C                                                 O2 dissolves in water if [O2] < its equilibrium value
          IF (XR(7) .LE. XE(7)) RATE(2) = RK(LU2,2)*(XE(7)-XR(7))
C                                                       only if O2 and CN- are present
          IF ((XR(7) .GT. ZERO) .AND. (XR(6) .GT. ZERO)) THEN
C                                                       CN- is oxydised to cyanate
            RATE(3) = RK(LU2,3)*XR(6)*XR(7)/XE(7)
C                                                       gold dissolves
            IF (XR(8) .GT. ZERO)
     &      RATE(4) = RK(LU2,4)*XR(8)/(6.316/XR(6) + 1/XR(7))
            IF (XR(9) .GT. ZERO)
     &      RATE(5) = RK(LU2,5)*XR(9)/(6.316/XR(6) + 1/XR(7))
C                                                       metal dissolves
            IF (XR(11) .GT. ZERO)
     &      RATE(6) = RK(LU2,6)*XR(11)/(9.81/XR(6) + 1/XR(7))
            IF (XR(12) .GT. ZERO)
     &      RATE(7) = RK(LU2,7)*XR(12)/(9.81/XR(6) + 1/XR(7))
          ENDIF
        ENDIF
C                                                 calculate derivatives of tank components
        DO 60 J=1,NCOMP
          DX(INX(L)+J) = ZERO
          DO 40 I=1,NSTRM
C                                                       add mols from any incoming stream
            IF (STREAM(I,2) .EQ. L) DX(INX(L)+J) = DX(INX(L)+J) +
     &                              A(INA(NUNIT+I)+J)
```

```
C                                                                  subtract mols for any leaving stream
      IF (STREAM(I,1) .EQ. L) DX(INX(L)+J) = DX(INX(L)+J) -
     &                              A(INA(NUNIT+I)+J)
40      CONTINUE

        IF (X(INX(L)+1) .GT. ZERO) THEN
          DO 50 K=1,NREAC
C                                                  rates are in terms of concentrations, thus multiply by liquid volume
            DX(INX(L)+J) = DX(INX(L)+J) + STOI(LU2,J,K)*RATE(K)*
     &             X(INX(L)+1)*CONV(LU2,1)*1000.
50        CONTINUE
          ENDIF
60      CONTINUE
        RETURN
        END

C ***********************************************************************
C                                                                       *
        SUBROUTINE DIF7(X,DX,NS,A,NA,T,L)
C                                                                       *
C       This is the subroutine to calculate the derivatives of the state *
C       variables associated with an adsorption tank.                   *
C                                                                       *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2,  NREAC = 12)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)
        PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

        DOUBLE PRECISION X,DX,A,T,TA,ZERO,CONV,XR,RATE,CON,XE
        DOUBLE PRECISION XAR,CR,CAR
        INTEGER UNIT, STREAM, CONN
        PARAMETER (ZERO = 0.0)
        DIMENSION X(NS),DX(NS),A(NA),XR(NCOMP),XE(NCOMP)
        DIMENSION RATE(NREAC),CON(NCOMP)

        COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
        COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
        COMMON /DIRIV/ STOI(NTYP2,NCOMP,NREAC),RK(NTYP2,NREAC)
        COMMON /CARBN/ FLO(NSTRM),HLA(NUNIT),HLD(NUNIT),ncond2

        TA = T
        LU1 = UNIT(L,1)
        LU2 = UNIT(L,2)
        DO 10 J=1,NCOMP
          CON(J) = ZERO
          XE(J) = ZERO
10      CONTINUE
        XE(4)  = 0.331E-06
        CON(9)  = 0.1*6.513E-06
        CON(10) = 0.9*6.513E-06
        CON(11) = 6.513E-06
        CON(12) = 0.1*1200.0E-06
        CON(13) = 0.9*1200.0E-06
        CON(14) = 1200.0E-06
        CON(16) = 0.1*1500.0E-06
        CON(17) = 0.9*1500.0E-06
        CON(18) = 1500.0E-06
        DO 20 K=1,NREAC
          RATE(K) = ZERO
20      CONTINUE

        IF (X(INX(L)+1) .GT. ZERO) THEN
```

```
      DO 30 J=1,NCOMP
C                                                  calculate concentrations ito liquid volumes (in kmol/l)
       XR(J) = X(INX(L)+J)/(X(INX(L)+1)*CONV(LU2,I)*1000.0)
30    CONTINUE
      CR = X(INX(L)+7)/475.5
C                                                  calculate rates of the chemical reactions :
      DO 40 K=1,3
       IF (K .EQ. 1) THEN
C                                                  for adsorption on carbon fines
        XAR = XR(8)
        CAR = 1.0
       ELSE
C                                                  for adsorption in meso- and micropores of coarse carbon
        XAR = XR(7)
        CAR = CR
       ENDIF
       IF (XAR .GT. ZERO) THEN
C                                                  Au(CN) adsorption
        RATE(K) = RK(LU2,K)*(XR(5) - CON(8+K)*XR(8+K)/XAR)*CAR
C                                                  M(CN) adsorption
        RATE(3+K)=RK(LU2,3+K)*(XR(6) - CON(11+K)*XR(11+K)/XAR)*CAR
C                                                  CN adsorption
        RATE(6+K)=RK(LU2,6+K)*(XR(3) - CON(14+K)*XR(14+K)/XAR)*CAR
       ENDIF
40    CONTINUE
C                                                  destruction of CN
      IF (XR(3) .GE. ZERO) RATE(10) = RK(LU2,10)*XR(3)*XR(4)/XE(4)
C                                                  carbon attrition
      IF (XR(7) .GE. ZERO) RATE(11) = RK(LU2,11)*XR(7)
      ENDIF
C                                                  calculate derivatives of tank components
      DO 70 J=1,NCOMP
       DX(INX(L)+J) = ZERO
       DO 50 I=1,NSTRM
C                                                  add mols from any incoming stream
        IF (STREAM(I,2) .EQ. L)
     &  DX(INX(L)+J) = DX(INX(L)+J) + A(INA(NUNIT+I)+J)
C                                                  subtract mols for any leaving stream
        IF ((STREAM(I,1) .EQ. L) .AND. (J .NE. 18))
     &  DX(INX(L)+J) = DX(INX(L)+J) - A(INA(NUNIT+I)+J)
50     CONTINUE
       IF (X(INX(L)+1) .GT. ZERO) THEN
        DO 60 K=1,NREAC
C                                                  rates are in terms of concentrations, thus multiply by liquid volumes
         DX(INX(L)+J) = DX(INX(L)+J) + STOI(LU2,J,K)*RATE(K)*
     &          X(INX(L)+1)*CONV(LU2,I)*1000.0
60      CONTINUE
       ENDIF
70    CONTINUE
      RETURN
      END

C ***************************************************************************
C                                                                            *
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C                                                                            *
C ***************************************************************************
```

I.4 ALGUS.F : ALGEBRAIC VARIABLES SUBROUTINES

```
C     THIS FILE CONTAINS ALL ALGEBRAIC ROUTINES FOR SIMU.FOR
C                                                                            *
C ***************************************************************************
C                                                                            *
      SUBROUTINE ALGU(X,NS,A,NA,T,I)
```

```
C                                                                       *
C       This  routine  calculates the  algebraic variables of any unit, *
C       with holdup :                                                   *
C     - the total number of mols and                                    *
C     - the total volume in the tank.                                   *
C                                                                       *
C ***********************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION MUNIT(NTYP1)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &       CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)

      TA = T
      LU2 = UNIT(I,2)
C                                                   zero mol total and total volume in tank
      DO 10 K=1,NTOTS
        A(INA(I)+K) = ZERO
10    CONTINUE
C                                                 then sum for mol total and total vol in tank
      DO 20 J=1,(NCOMP-1)
C                                                   (but don't include the transferred carbon)
        A(INA(I)+1) = A(INA(I)+1) + X(INX(I)+J)
        A(INA(I)+2) = A(INA(I)+2) + X(INX(I)+J)*CONV(LU2,J)
20    CONTINUE
      KALG(I) = 1
      RETURN
      END

C ***********************************************************************
C                                                                       *
      SUBROUTINE ALGS1(X,NS,A,NA,T,I,L)
C                                                                       *
C       This is the subroutine to calculate the algebraic  variables of *
C       the exit stream of a feeder unit.                               *
C                                                                       *
C ***********************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,ONE,CONV,DLIQ,DSOL
      DOUBLE PRECISION DTOT,WLIQ,WSOL,WTOT,VSOL,VTOT
      DOUBLE PRECISION VFRS,WFRP,VFEED,VLIME,VCYAR,VCYAN
      DOUBLE PRECISION VLFRC,VCFRC,TRLIMIT,CCLIMIT
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0, ONE = 1.0)
      DIMENSION X(NS),A(NA)
      DIMENSION VFRS(NCOMP),WFRP(NCOMP)
      DIMENSION MUNIT(NTYP1)
```

```
      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)
      COMMON /CARBN/ FLO(NSTRM),IBLK(NUNIT)
      COMMON /FEEDS/ OPTSIM,DAT(18),LUAT
      COMMON /OPTNS/ OPT2,OPT3,TRLIMIT,OPT4,CCLIMIT,NCOND2,
     &          OPT5,OPT6,OPT7,OPT8,OPT9

      TA = T
      LU2 = UNIT(L,2)

      IF ((OPTSIM .EQ. '1') .OR. (OPTSIM .EQ. '2')) THEN
       IF ((L .EQ. 4) .AND. (A(INA(NUNIT+3)+1).EQ. ZERO)) THEN
C                                                    CN-stream starts flowing only if tank 3 overflows
        DO 10 J=1,NCOMP+NTOTS
         A(INA(NUNIT+I)+J) = ZERO
10      CONTINUE
       ELSEIF ((L .EQ. 5) .AND. ((A(INA(NUNIT+3)+1) .EQ. ZERO) .OR.
     &                (LUAT .EQ. 0))) THEN
C                                          Eluate stream flows only if tank 3 overflows and it is turned on
        DO 20 J=1,NCOMP+NTOTS
         A(INA(NUNIT+I)+J) = ZERO
20      CONTINUE
       ELSEIF (L .EQ. 27) THEN
C                                                    calculate amts added in regenerated carbon transfer
        DO 30 J=1,NCOMP+NTOTS
         A(INA(NUNIT+I)+J) = ZERO
30      CONTINUE
        IF ((FLO(35).EQ.1.0) .AND. (IBLK(28) .EQ. 0)) THEN
         IF (OPT2.NE.'3') THEN
          IF ((X(INX(28)+18).LT.TRLIMIT) .OR. ((OPT4.EQ.'1') .AND.
     &    (NCOND2.EQ.1) .AND. (X(INX(28)+7) .LT. CCLIMIT))) THEN
           DO 40 J=1,NCOMP
            IF (J .NE. 18) THEN
             A(INA(NUNIT+I)+J) = X(INX(L)+J)
            ENDIF
40          CONTINUE
            A(INA(NUNIT+I)+18) = A(INA(NUNIT+I)+7)
          ENDIF
         ELSE
C                                                    for continuous transfer, reduce flowrate of fresh carbon
          IF (OPT3 .EQ. '1') THEN
           FACT = 1.0
          ELSE
           FACT = 0.5
          ENDIF
          DO 50 J=1,NCOMP
           IF (J.EQ.1) THEN
            A(INA(NUNIT+I)+J) = X(INX(L)+J)*0.1117362*FACT
           ELSEIF (J.EQ.7) THEN
            A(INA(NUNIT+I)+J) = X(INX(L)+J)*0.1117362*FACT
           ELSEIF (J.EQ.18) THEN
            A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+7)
           ELSE
            A(INA(NUNIT+I)+J) = X(INX(L)+J)
           ENDIF
50        CONTINUE
         ENDIF
        ENDIF
       ELSE
        DO 60 J=1,NCOMP
         A(INA(NUNIT+I)+J) = X(INX(L)+J)
60      CONTINUE
        DO 70 J=1,NTOTS
         A(INA(NUNIT+I)+NCOMP+J) = A(INA(L)+J)
70      CONTINUE
```

```
      ENDIF
     ELSE
C                                                                  for optsim = 3
      DO 80 J=1,NCOMP+NTOTS
       A(INA(NUNIT+I)+J)=ZERO
80    CONTINUE
      IF (L .EQ. 1) THEN
C                                                                  for the pulp feed stream
       IF (OPT6 .EQ. '1') THEN
        DO 90 J=1, NCOMP
         A(INA(NUNIT+I)+J) = X(INX(L)+J)
90      CONTINUE
        DO 100 J=1,NTOTS
         A(INA(NUNIT+I)+NCOMP+J) = A(INA(L)+J)
100     CONTINUE
       ELSE
C                                                  calculate total mass and solid mass and volume
        WTOT = ZERO
        WSOL = ZERO
        VSOL = ZERO
        DO 110 J=1,NCOMP
         WTOT = WTOT + X(INX(L)+J)*PHYS(LU2,J,1)
         IF ((J .NE. 1) .AND. (CONV(LU2,J) .NE. ZERO)) THEN
          VSOL = VSOL + X(INX(L)+J)*CONV(LU2,J)
          WSOL = WSOL + X(INX(L)+J)*PHYS(LU2,J,1)
         ENDIF
110     CONTINUE
        DO 120 J=1,NCOMP
         IF (WTOT .NE. ZERO) THEN
C                                          calculate individual mass fractions for all components
          WFRP(J) = X(INX(L)+J)*PHYS(LU2,J,1)/WTOT
         ENDIF
         IF ((J .NE. 1) .AND. (CONV(LU2,J) .NE. ZERO) .AND.
     &      (VSOL .NE. ZERO)) THEN
C                                                          calculate solid volume fractions
          VFRS(J) = X(INX(L)+J)*CONV(LU2,J)/VSOL
         ENDIF
120     CONTINUE
C                                                  calculate liquid, solid and total densities
        DLIQ = PHYS(LU2,1,2)
        DSOL = WSOL/VSOL
        DTOT = DAT(9)*1000.0
C                                                                  => tot density in kg/m3
        FRL = (DSOL-DTOT)/(DSOL-DLIQ)
C                                                                  => mass fraction of liq
        VTOT = (DAT(7)/3600.0)*(194.4688/173.47)
C                                                                  => pulp flow in m3/s

        DO 130 J=1,NCOMP
C                                                  calculate mols of each substance in pulp stream :
         IF (J .EQ. 1) THEN
C                                                                  - for water
          A(INA(NUNIT+I)+J) = FRL*VTOT/CONV(LU2,1)
         ELSEIF (CONV(LU2,J) .EQ. ZERO) THEN
C                                                                  - for dissolved substs
          A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &                        X(INX(L)+1)
         ELSE
C                                                                  - for solid components
          A(INA(NUNIT+I)+J) = (1-FRL)*VTOT*VFRS(J)/CONV(LU2,J)
         ENDIF
130     CONTINUE
       ENDIF

      ELSEIF (L .EQ. 2) THEN
C                                                  calculate amounts added in lime stream
       IF (OPT7 .EQ. '1') THEN
```

```
            DO 140 J=1,NCOMP
              A(INA(NUNIT+I)+J) = X(INX(L)+J)
140         CONTINUE
C                                                          add lime in proportion to feed
           ELSE
            VLIME = ZERO
            VFEED = ZERO
            VTOT = (DAT(7)/3600.0)*(194.4688/173.47)
            DO 150 J=1,NCOMP
              VLIME = VLIME + X(INX(L)+J)*CONV(LU2,J)
              VFEED = VFEED + X(INX(1)+J)*CONV(LU2,J)
150         CONTINUE
            DO 160 J=1,NCOMP
              IF (CONV(LU2,J) .NE. ZERO) THEN
                VLFRC = X(INX(L)+J)*CONV(LU2,J)/VLIME
                A(INA(NUNIT+I)+J) =
     &                VLFRC*VLIME*VTOT/(VFEED*CONV(LU2,J))
              ELSE
                A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &                  X(INX(L)+1)
              ENDIF
160         CONTINUE
           ENDIF

          ELSEIF (L .EQ. 4) THEN
C                                                          calculate amts added in CN stream
           IF (OPT8 .EQ. '1') THEN
C                                                          option 1 : add const amt of CN
            DO 170 J=1,NCOMP
              A(INA(NUNIT+I)+J) = X(INX(L)+J)
170         CONTINUE
C                                                          option 2 : add cyanide in proportion to feed
           ELSEIF (OPT8 .EQ. '2') THEN
            VCYAN = ZERO
            VFEED = ZERO
            VTOT = (DAT(7)/3600.0)*(194.4688/173.47)
            DO 180 J=1,NCOMP
              VCYAN = VCYAN + X(INX(L)+J)*CONV(LU2,J)
              VFEED = VFEED + X(INX(1)+J)*CONV(LU2,J)
180         CONTINUE
            DO 190 J=1,NCOMP
              IF (CONV(LU2,J) .NE. ZERO) THEN
                VCFRC = X(INX(L)+J)*CONV(LU2,J)/VCYAN
                A(INA(NUNIT+I)+J) =
     &                VCFRC*VCYAN*VTOT/(VFEED*CONV(LU2,J))
              ELSE
                A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &                  X(INX(L)+1)
              ENDIF
190         CONTINUE
           ELSE
C                                                          option 3 : add CN according to recorded plant data
            VCYAR = DAT(1)/(1000.0*3600.0)
C                                                          => CN flow in m3/s
            VCYAN = ZERO
            DO 200 J=1,NCOMP
              VCYAN = VCYAN + X(INX(L)+J)*CONV(LU2,J)
200         CONTINUE
            DO 210 J=1,NCOMP
              IF (VCYAN .GT. ZERO) THEN
                A(INA(NUNIT+I)+J) = X(INX(L)+J)*VCYAR/VCYAN
              ENDIF
210         CONTINUE
           ENDIF

          ELSEIF (L .EQ. 5) THEN
C                                                          calculate amts added in spent eluate
```

```
          IF (LUAT .EQ. 1) THEN
           DO 220 J=1,NCOMP
            A(INA(NUNIT+I)+J) = X(INX(L)+J)
220         CONTINUE
          ENDIF

         ELSEIF (L .EQ. 27) THEN
C                                                    calculate amts added in regenerated carbon transfer
          IF ((FLO(35).EQ.1.0) .AND. (IBLK(28) .EQ. 0)) THEN
           IF (OPT2.NE.'3') THEN
            IF ((X(INX(28)+18).LT.TRLIMIT) .OR. ((OPT4.EQ.'1') .AND.
     &       (NCOND2.EQ.1) .AND. (X(INX(28)+7) .LT. CCLIMIT))) THEN
             DO 230 J=1,NCOMP
              IF (J .NE. 18) THEN
               A(INA(NUNIT+I)+J) = X(INX(L)+J)
              ENDIF
230           CONTINUE
              A(INA(NUNIT+I)+18) = A(INA(NUNIT+I)+7)
             ENDIF
            ELSE
C                                                    for continuous transfer, reduce addn of fresh carbon
             IF (OPT3 .EQ. '1') THEN
              FACT = 1.0
             ELSE
              FACT = 0.5
             ENDIF
             DO 240 J=1,NCOMP
              IF (J.EQ.1) THEN
               A(INA(NUNIT+I)+J) = X(INX(L)+J)*0.1117362*FACT
              ELSEIF (J.EQ.7) THEN
               A(INA(NUNIT+I)+J) = X(INX(L)+J)*0.1117362*FACT
              ELSEIF (J.EQ.18) THEN
               A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+7)
              ELSE
               A(INA(NUNIT+I)+J) = X(INX(L)+J)
              ENDIF
240           CONTINUE
            ENDIF
           ENDIF
          ENDIF

C                                                    calculate mol total and total volume
          DO 250 J=1,NCOMP
           IF (J .NE. 18) THEN
            A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &                  A(INA(NUNIT+I)+J)
            A(INA(NUNIT+I)+NCOMP+2) = A(INA(NUNIT+I)+NCOMP+2) +
     &                  A(INA(NUNIT+I)+J)*CONV(LU2,J)
           ENDIF
250        CONTINUE
          ENDIF
          KALG(NUNIT+I) = 1
          RETURN
          END

C ***************************************************************************
C                                                                            *
          SUBROUTINE ALGS3(X,NS,A,NA,T,I,L)
C                                                                            *
C         This routine calculates the algebraic variables of stream I        *
C         leaving distributor box L:                                         *
C         - the number of mols of each component in the stream,              *
C         - the total number of mols in the stream, and                      *
C         - the total volume taken up by the stream.                         *
C                                                                            *
C ***************************************************************************
```

```
      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION MUNIT(NTYP1)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &       CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)

      TA = T
      LU2 = UNIT(L,2)
C                                                    zero mol total and total volume out of box
      DO 10 K=1,(NCOMP+NTOTS)
        A(INA(NUNIT+I)+K) = ZERO
10    CONTINUE

      DO 30 M=1,NSTRM
        IF (STREAM(M,2) .EQ. L) THEN
          DO 20 J=1,NCOMP
C                                                    calculate individual molar flows out of box
            A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+J) + A(INA(NUNIT+M)+J)
20        CONTINUE
        ENDIF
30    CONTINUE
      DO 40 J=1,NCOMP
C                                                    sum for total flow and total volume
        A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &            A(INA(NUNIT+I)+J)
        A(INA(NUNIT+I)+NCOMP+2) = A(INA(NUNIT+I)+NCOMP+2) +
     &            A(INA(NUNIT+I)+J)*CONV(LU2,J)
40    CONTINUE
      KALG(NUNIT+I) = 1
      RETURN
      END

C ***************************************************************************
C                                                                            *
      SUBROUTINE ALGS4(X,NS,A,NA,T,I,L)
C                                                                            *
C     This routine calculates the algebraic variables of both the            *
C     streams leaving a screen. Automatically the first stream en-           *
C     countered is assumed to be the underflow, while the second one         *
C     is the overflow. Variables calculated are :                            *
C     - the number of mols of each component in the stream,                  *
C     - the total number of mols in the stream, and                          *
C     - the total volume taken up by the stream.                             *
C                                                                            *
C ***************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                  + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV
      INTEGER UNIT, STREAM, CONN
```

```
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION MUNIT(NTYP1)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &        CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)
      COMMON /SCREN/ NOONE

      TA = T
      LU2 = UNIT(L,2)
C                                                    zero mol total and total volume out of screen
      DO 10 J=1,NCOMP+NTOTS
        A(INA(NUNIT+I)+J) = ZERO
10    CONTINUE

      DO 40 M=1,NSTRM
        IF (STREAM(M,2) .EQ. L) THEN
          IF (NOONE .EQ. 1) THEN
C                                                    for the underflow calculate molar flows out of screen
            DO 20 J=1,NCOMP
C                                                    this stream contains no coarse carbon
              IF ((J .NE. 7) .AND. (J .NE. 10) .AND. (J .NE. 11) .AND.
     &        (J .NE. 13) .AND. (J .NE. 14) .AND. (J .NE. 16) .AND.
     &        (J .NE. 17) .AND. (J .NE. 18)) THEN
                A(INA(NUNIT+I)+J) = A(INA(NUNIT+M)+J)
              ENDIF
20          CONTINUE
            A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+M)+NCOMP+1) -
     &                  A(INA(NUNIT+M)+7)
            A(INA(NUNIT+I)+NCOMP+2) = A(INA(NUNIT+M)+NCOMP+2) -
     &                  A(INA(NUNIT+M)+7)*CONV(LU2,7)
            NOONE = 0
          ELSE
C                                                    the overflow contains only coarse carbon
            DO 30 J=1,NCOMP
              IF ((J .EQ. 7) .OR. (J .EQ. 10) .OR. (J .EQ. 11) .OR.
     &        (J .EQ. 13) .OR. (J .EQ. 14) .OR. (J .EQ. 16) .OR.
     &        (J .EQ. 17)) A(INA(NUNIT+I)+J) = A(INA(NUNIT+M)+J)
              IF (J .EQ. 18) A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+7)
30          CONTINUE
            A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+7)
            A(INA(NUNIT+I)+NCOMP+2) =
     &                  A(INA(NUNIT+I)+7)*CONV(LU2,7)
            NOONE = 1
          ENDIF
        ENDIF
40    CONTINUE
      KALG(NUNIT+I) = 1
      RETURN
      END

C ***************************************************************************
C                                                                            *
      SUBROUTINE ALGS5(X,NS,A,NA,T,I,L)
C                                                                            *
C     This routine calculates the algebraic variables of stream I            *
C     leaving a general tank L :                                             *
C     - the number of mols of each component in the stream,                  *
C     - the total number of mols in the stream, and                          *
C     - the total volume taken up by the stream.                             *
C                                                                            *
C ***************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
```

```
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                 + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV,VFR,DV,AREA,HALFHT
     DOUBLE PRECISION VMAX
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION VFR(NCOMP)
      DIMENSION MUNIT(NTYP1)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2)
     &       CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)

      TA    = T
      PI    = 3.1415926536
      AREA  = PI*(4.5)**2
      HALFHT = 9.22/2
      VMAX  = AREA*HALFHT

      LU2 = UNIT(L,2)
C                                                    zero mol total and total volume out of tank
      DO 10 K=1,NCOMP+NTOTS
        A(INA(NUNIT+I)+K) = ZERO
10    CONTINUE
      DV = ZERO

      IF (A(INA(L)+2) .GT. VMAX) THEN
        DV = 0.01*(A(INA(L)+2) - VMAX)
        IF (DV .GT. A(INA(L)+2)) DV = A(INA(L)+2)

        DO 20 J=1,NCOMP
C                                                    calculate volume fraction VFR of each component
          VFR(J) = X(INX(L)+J) * CONV(LU2,J) / A(INA(L)+2)
C                                                    calculate individual molar flows out of tank
          IF (CONV(LU2,J).NE.ZERO) THEN
C                                                    for components with volume use volume fractions
            A(INA(NUNIT+I)+J) = DV*VFR(J)/CONV(LU2,J)
          ELSE
C                                                    for dissolved species, flow out is proportional to water
            A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &                  X(INX(L)+1)
          ENDIF
C                                                    and sum for total flow
          A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &                    A(INA(NUNIT+I)+J)
20      CONTINUE
C                                                    calculate total volume out of tank
        A(INA(NUNIT+I)+NCOMP+2) = DV
      ENDIF
      KALG(NUNIT+I) = 1
      RETURN
      END

C ***************************************************************************
C                                                                            *
      SUBROUTINE ALGS6(X,NS,A,NA,T,I,L)
C                                                                            *
C     This routine  calculates the algebraic  variables of  stream I         *
C     leaving leach pachuca L:                                               *
C     - the number of mols of each component in the stream,                  *
C     - the total number of mols in the stream, and                          *
C     - the total volume taken up by the stream.                             *
```

```
C                                                                       *
C ***********************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                 + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV,VFR,DV
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION VFR(NCOMP),LON(NUNIT)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &       CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)
      COMMON /UNICO/ MUNIT(NTYP1),LUNIT

      TA  = T
      PI  = 3.1415926536
      AREA = PI*(4.5**2)

      LU2 = UNIT(L,2)
      LUNIT = LUNIT + 1
      IF (LUNIT .EQ. MUNIT(6)) THEN
       VMAX = AREA*18.0
      ELSE
       VMAX = AREA*16.9
      ENDIF
C                                                  zero mols, mol total and total vol out of tank
      DO 10 K=1,NCOMP+NTOTS
       A(INA(NUNIT+I)+K) = ZERO
10    CONTINUE
      DV = ZERO

      IF (A(INA(L)+2) .GT. ZERO) THEN
       LSON = 0
       DO 20 M=1,NSTRM
        IF (STREAM(M,2) .EQ. L) LSON = 1
20     CONTINUE
       IF (LSON .EQ. 0) THEN
C                                        if no stream flows into tank L, empty it at constant flow
        DV = VMAX/(3600.0*24.0)
        IF (DV .GT. A(INA(L)+2)) DV = A(INA(L)+2)
       ELSEIF (A(INA(L)+2) .GT. VMAX) THEN
C                                        otherwise, only if tank overflows, calculate exit stream
        IF ((LUNIT .EQ. MUNIT(6)) .OR.
     &      (A(INA(STREAM(I,2))+2) .LT. VMAX)) THEN
C                                        tank L is the last in line, or the next tank is too empty
         DV = 0.01*(A(INA(L)+2) - VMAX)
        ELSE
C                                        if levels of tank L and L+1 interact
         DV = 0.01*(A(INA(L)+2)-A(INA(L+1)+2))
        ENDIF
       ENDIF
       IF (DV .GT. ZERO) THEN
        DO 30 J=1,NCOMP
C                                        calculate volume fraction VFR of each component
         VFR(J) = X(INX(L)+J) * CONV(LU2,J) / A(INA(L)+2)
C                                        calculate individual molar flows out of tank
         IF (CONV(LU2,J).NE.ZERO) THEN
C                                        for compts with volume use volume fractions
          A(INA(NUNIT+I)+J) = DV*VFR(J)/CONV(LU2,J)
```

```
            ELSE
C                                                    for dissolved species, flow out is proportional to water
              A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &                    X(INX(L)+1)
            ENDIF
C                                                    and sum for total flow
          A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &                       A(INA(NUNIT+I)+J)
30          CONTINUE
C                                                    calculate total volume out of tank
            A(INA(NUNIT+I)+NCOMP+2) = DV
          ENDIF
        ENDIF
        KALG(NUNIT+I) = 1
        RETURN
        END

C ***********************************************************************
C                                                                      *
        SUBROUTINE ALGS7(X,NS,A,NA,T,I,L)
C                                                                      *
C       This routine  calculates the algebraic  variables of streams I *
C       leaving CIP contactor L. The composition of the stream depends *
C       on whether it is a pulp stream or a carbon transfer stream.    *
C       Find - the number of mols of each component in the stream,     *
C           - the total number of mols in the stream, and              *
C           - the total volume taken up by the stream.                 *
C                                                                      *
C ***********************************************************************

        PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
        PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2, NADS = 8)
        PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                   + NCONN*2)
        PARAMETER (NSTAT = NUNIT*NCOMP)
        PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

        DOUBLE PRECISION X,A,T,ZERO,PI,CONV,VFR,DV,TAREA,SAREA
        DOUBLE PRECISION AAREA,PAREA,CLEAK,CFLO,ACVOL,VMIN
        DOUBLE PRECISION VOVR,VANN,VSCR,VMAX,TRLIMIT,CCLIMIT
        INTEGER UNIT, STREAM, CONN
        PARAMETER (ZERO = 0.0, PI = 3.1415926536)
        DIMENSION X(NS),A(NA)
        DIMENSION VFR(NCOMP),CFLO(NSTRM)
        DIMENSION MUNIT(NTYP1)

        COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &          CONN(NCONN,2),INX(NUNIT),INA(NPROC)
        COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
        COMMON /ALALG/ KALG(NPROC)
        COMMON /CARBN/ FLO(NSTRM),IBLK(NUNIT)
        COMMON /FEEDS/ OPTSIM,DAT(18),LUAT
        COMMON /OPTNS/ OPT2,OPT3,TRLIMIT,OPT4,CCLIMIT,NCOND2,
     &          OPT5,OPT6,OPT7,OPT8,OPT9

        TA   = T
        HSCR  = 5.3
        HTRN  = 4.8
        HTNK  = 6.0
        DC    = 7.0
        DS    = 3.9
        DSA   = 3.6
        DP    = 0.11
        TAREA = PI*(DC/2)**2
        SAREA = PI*(DS/2)**2
        AAREA = PI*(DSA/2)**2
        PAREA = PI*(DP/2)**2
```

```
      VMIN  = TAREA*HTRN
      VOVR  = TAREA*HSCR
      VANN  = (TAREA - SAREA)*(HTNK - HSCR)
      VSCR  = SAREA*(HTNK - HSCR)
      VMAX  = VOVR + VANN
      IF (OPT5 .EQ. '1') THEN
       CLEAK = 0.001*X(INX(L)+7)
      ELSE
       CLEAK = ZERO
      ENDIF
C                                                    0.1% of coarse carbon in tank leaks into pulp stream
      FAC   = 0.02
      RES   = 0.03

      LU2 = UNIT(L,2)
      IF ((OPT2.EQ.'1') .OR. (OPT2.EQ.'2')) THEN
       CFLO(18) = PAREA*3.0
       DO 10 J=1,7
        CFLO(J*2+19) = PAREA*3.0
10     CONTINUE
      ELSEIF (OPT2 .EQ. '3') THEN
       IF (OPT3 .EQ. '1') THEN
        FACT = 1.0
       ELSE
        FACT = 0.5
       ENDIF
       CFLO(18) = PAREA*0.3299*FACT
       DO 20 J=1,7
        CFLO(J*2+19) = PAREA*0.3299*FACT
20     CONTINUE
      ELSE
       CFLO(18) = PAREA*0.75
       CFLO(21) = PAREA*1.14
       CFLO(23) = PAREA*2.12
       CFLO(25) = PAREA*3.12
       CFLO(27) = PAREA*2.92
       CFLO(29) = PAREA*2.72
       CFLO(31) = PAREA*2.80
       CFLO(33) = PAREA*2.16
      ENDIF

      DO 30 M=1,NSTRM
       IF ((FLO(M) .EQ. 0.0) .OR. (IBLK(STREAM(M,1)).NE.0) .OR.
     &  (IBLK(STREAM(M,2)).NE.0)) THEN
        CFLO(M) = ZERO
       ELSEIF ((OPT2 .NE.'3') .AND. (OPT9.NE.'3')) THEN
        IF ((OPT4.EQ.'Y') .AND. (NCOND2 .EQ.'1')) THEN
         IF (STREAM(M,2) .EQ. 19) THEN
          IF (X(INX(20)+7) .GE. CCLIMIT) CFLO(M) = ZERO
         ELSE
          IF (X(INX(STREAM(M,2))+7) .GE. CCLIMIT) CFLO(M) = ZERO
         ENDIF
        ELSE
         IF (STREAM(M,2) .EQ. 19) THEN
          IF (X(INX(20)+18) .GE. TRLIMIT) CFLO(M)= ZERO
         ELSE
          IF (X(INX(STREAM(M,2))+18) .GE. TRLIMIT) CFLO(M)= ZERO
         ENDIF
        ENDIF
       ENDIF
30     CONTINUE
C                                                    zero mol total and total volume out of tank
      DO 40 K=1,NCOMP+NTOTS
       A(INA(NUNIT+I)+K) = ZERO
40     CONTINUE
      DV = ZERO
```

```
      IF (IBLK(L) .EQ. 0) THEN
C                                                          the screen is not blocked
       IF ((STREAM(I,2) .EQ. STREAM(I+1,1)) .AND.
     &  (STREAM(I+1,2) .EQ. L)) THEN
C                                                          this is a carbon transfer stream
        IF ((A(INA(L)+2) .GT. VMIN) .AND. (CFLO(I) .GT. ZERO)) THEN
         KARBON = 1
         DV = CFLO(I)
         ACVOL = A(INA(L)+2)
        ENDIF
       ELSE
C                                                          this is a pulp stream
        IF ((A(INA(L)+2).GT.VOVR).AND. (IBLK(STREAM(I,2)) .NE.2)) THEN
C                                                          which normally contains little carbon
         KARBON = 0
         ACVOL = A(INA(L)+2) - (X(INX(L)+7) - CLEAK)*CONV(LU2,7)
         DV = FAC*(SAREA/AAREA)*(A(INA(L)+2) - VOVR)
         DO 50 M=1,NSTRM
          IF ((STREAM(M,1) .EQ. L) .AND.
     &     (STREAM(M,2) .EQ. STREAM(M+1,1))) THEN
C                                                          this is the corresponding transfer stream
           IF (CFLO(M) .GT. ZERO) DV = DV - CFLO(M)
C                                                          subtract volume of carbon transfer stream
           IF (DV .LT. ZERO) DV = ZERO
          ENDIF
50        CONTINUE
        ENDIF
       ENDIF
      ELSEIF (IBLK(L) .EQ. 1) THEN
C                                                          the screen is blocked
       IF ((STREAM(I,2) .EQ. STREAM(I+1,1)) .AND.
     &  (STREAM(I+1,2) .EQ. L)) THEN
C                                                          no transfer stream leaves the tank
        DV = ZERO
       ELSE
        IF (A(INA(L)+2) .LT. (VMAX +VSCR)) THEN
         print *,'volm =',a(ina(l)+2),'  vmx+vsc=',(VMAX+VSCR)
C                                                          no pulp stream leaves the tank
         DV = ZERO
        ELSE
C                                                          unless the screen has filled and flow out starts
         KARBON = 1
         ACVOL = A(INA(L)+2)
         DV = FAC*(SAREA/(TAREA-SAREA))*(A(INA(L)+2) - VMAX)
C                                                          but then pulp stream into tank must be cut
         DO 60 J=1,NCOMP+NTOTS
          IF (L .EQ. 18) THEN
           A(INA(NUNIT+I-2)+J) = ZERO
          ELSE
           A(INA(NUNIT+I-1)+J) = ZERO
          ENDIF
60        CONTINUE
         IF (L .EQ. 18) THEN
          KALG(NUNIT+I-2) = 1
         ELSE
          KALG(NUNIT+I-1) = 1
         ENDIF
        ENDIF
       ENDIF
      ELSE
C                                                          IBLK(L) = 2
       IF (A(INA(L)+2) .GT. VMAX) THEN
C                                                          the screen is eptying; C is carried along
        IF (L .EQ. 18) THEN
C                                                          ensure that no pulp enters blocked first CIP tank
         DO 70 J=1,NCOMP+NTOTS
          A(INA(NUNIT+I-2)+J) = ZERO
```

```
            A(INA(NUNIT+I-1)+J) = ZERO
70          CONTINUE
            KALG(NUNIT+I-2) = 1
            KALG(NUNIT+I-1) = 1
           ENDIF
           KARBON = 1
           ACVOL = A(INA(L)+2)
           DV = FAC*(SAREA/(TAREA-SAREA))*(A(INA(L)+2) -
     &    0.5*(VMAX+VOVR))
           ELSE
C                                                                    back to normal operation
           KARBON = 0
           ACVOL = A(INA(L)+2) - (X(INX(L)+7) - CLEAK)*CONV(LU2,7)
           DV = FAC*(SAREA/AAREA)*(A(INA(L)+2) - VOVR)
          ENDIF
         ENDIF

         IF (DV .GT. ZERO) THEN
          DO 80 J=1,NCOMP
C                                                  calculate volume fraction VFR of each component
           IF ((KARBON .EQ. 0) .AND. (J .EQ. 7)) THEN
            VFR(J) = CLEAK*CONV(LU2,J)/ACVOL
           ELSE
            VFR(J) = X(INX(L)+J) * CONV(LU2,J) / ACVOL
           ENDIF
C                                                      calculate individual molar flows out of tank
           IF (CONV(LU2,J) .NE. ZERO) THEN
            A(INA(NUNIT+I)+J) = DV*VFR(J)/CONV(LU2,J)
C                                    all amts of adsorbed species are proportional to amt of carbon
           ELSEIF (((J .EQ. 9) .OR. (J .EQ. 12) .OR. (J .EQ. 15)) .AND.
     &          (X(INX(L)+8) .GT. ZERO)) THEN
            A(INA(NUNIT+I)+J) =
     &          A(INA(NUNIT+I)+8)*X(INX(L)+J)/X(INX(L)+8)
           ELSEIF (((J .EQ. 10) .OR. (J .EQ. 11) .OR. (J .EQ. 13) .OR.
     &          (J .EQ. 14) .OR. (J .EQ. 16) .OR. (J .EQ. 17)) .AND.
     &          (X(INX(L)+7) .GT. ZERO)) THEN
            A(INA(NUNIT+I)+J) =
     &          A(INA(NUNIT+I)+7)*X(INX(L)+J)/X(INX(L)+7)
           ELSEIF (J .NE. 18) THEN
C                                          for dissolved species, flow out is proportional to water
            A(INA(NUNIT+I)+J) = A(INA(NUNIT+I)+1)*X(INX(L)+J)/
     &          X(INX(L)+1)
           ENDIF
C                                                                    and sum for total flow
           A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &          A(INA(NUNIT+I)+J)
80        CONTINUE
C                                                          calculate total volume out of tank
          A(INA(NUNIT+I)+NCOMP+2) = DV
C                                                  the carbon transferred must'nt be added twice
       IF ((KARBON .EQ. 1) .AND. (STREAM(I,2) .EQ. STREAM(I+1,1)) .AND.
     &  (STREAM(I+1,2).EQ. L))
     &          A(INA(NUNIT+I)+18) = A(INA(NUNIT+I)+7)
          ENDIF
          KALG(NUNIT+I) = 1
          RETURN
          END

C ***************************************************************************
C                                                                             *
          SUBROUTINE ALGS8(X,NS,A,NA,T,I,L)
C                                                                             *
C         This routine rearranges the components in the stream between        *
C         the leach and CIP cascades. This is necessary as the carbon         *
C         and loading terms for the ions on the carbon are not needed in      *
C         the leach, and leaching is assumed to be completed before CIP.      *
C          Components in leach :              Components in CIP :             *
```

```
C       1 : H2O                         1 : H2O                         *
C       2 : SiO                         2 : SiO2                        *
C       3 : Ca(OH)2                     3 : CN-                         *
C       4 : Ca++                        4 : O2 (aq)                     *
C       5 : OH-                         5 : Au(CN)2-                    *
C       6 : CN-                         6 : M(CN)3=                     *
C       7 : O2 (aq)                     7 : Carbon Granules             *
C       8 : Au-f                        8 : Carbon Fines                *
C       9 : Au-s                        9 : G-Au-fin                    *
C       10 : Au(CN)2-                   10 : G-Au-s                     *
C       11 : M-f                        11 : G-Au-f                     *
C       12 : M-s                        12 : G-M-fin                    *
C       13 : M(CN)3=                    13 : G-M-s                      *
C                                       14 : G-M-f                      *
C                                       15 : G-CN-fin                   *
C                                       16 : G-CN-s                     *
C                                       17 : G-CN-f                     *
C                                       18 : Total Carbon Transfd       *
C ***************************************************************************

      PARAMETER (NUNIT = 30, NSTRM = 40, NCONN = 40, NTYP1 = 9)
      PARAMETER (NTYP2 = 2,  NCOMP = 18, NTOTS = 2)
      PARAMETER (NALGB = NUNIT*NTOTS + NSTRM*(NTOTS+NCOMP)
     &                 + NCONN*2)
      PARAMETER (NSTAT = NUNIT*NCOMP)
      PARAMETER (NPROC = NUNIT + NSTRM + NCONN)

      DOUBLE PRECISION X,A,T,ZERO,CONV
      INTEGER UNIT, STREAM, CONN
      PARAMETER (ZERO = 0.0)
      DIMENSION X(NS),A(NA)
      DIMENSION MUNIT(NTYP1)

      COMMON /TOALL/ UNIT(NUNIT,2),STREAM(NSTRM,2),
     &       CONN(NCONN,2),INX(NUNIT),INA(NPROC)
      COMMON /DINAL/ PHYS(NTYP2,NCOMP,2),CONV(NTYP2,NCOMP)
      COMMON /ALALG/ KALG(NPROC)
      COMMON /MNNDV/ KALLS

      TA = T
      LU2 = UNIT(L,2)
C                                                   zero mol total and total vol out of tank
      DO 10 J=1,NCOMP+NTOTS
        A(INA(NUNIT+I)+J) = ZERO
10    CONTINUE

      DO 20 M=1,NSTRM
        IF (STREAM(M,2) .EQ. L) THEN
          A(INA(NUNIT+I)+1) = A(INA(NUNIT+M)+1)
          A(INA(NUNIT+I)+2) = A(INA(NUNIT+M)+2)
          A(INA(NUNIT+I)+3) = A(INA(NUNIT+M)+6)
          A(INA(NUNIT+I)+4) = A(INA(NUNIT+M)+7)
          A(INA(NUNIT+I)+5) = A(INA(NUNIT+M)+10)
          A(INA(NUNIT+I)+6) = A(INA(NUNIT+M)+13)
        ENDIF
20    CONTINUE
      DO 30 J=1,NCOMP
        IF (CONV(LU2,J) .NE. ZERO) THEN
C                                                   sum for total flow and total volume
          A(INA(NUNIT+I)+NCOMP+1) = A(INA(NUNIT+I)+NCOMP+1) +
     &                A(INA(NUNIT+I)+J)
          A(INA(NUNIT+I)+NCOMP+2) = A(INA(NUNIT+I)+NCOMP+2) +
     &                A(INA(NUNIT+I)+J)*CONV(LU2,2)
        ENDIF
30    CONTINUE
      KALG(NUNIT+I) = I
      RETURN
```

```
      END

C ***************************************************************************
C                                                                           *
C       Copyright (c) MINTEK 1992. Right of Reproduction Reserved.          *
C                                                                           *
C ***************************************************************************
```

I.5 CHEM.DAT : CHEMICAL DATA FILE

Stoichiometric Constants for Leach Reactions :

```
 0.0  0.0  0.0 -0.955 -0.955 -1.835 -1.835  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
-1.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 1.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 2.0  0.0  0.0  1.000  1.000  1.000  1.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0 -1.0 -2.000 -2.000 -4.000 -4.000  0.0  0.0  0.0  0.0  0.0
 0.0  1.0 -0.5 -0.478 -0.478 -0.917 -0.917  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0 -1.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000 -1.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  1.000  1.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000 -1.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000 -1.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  1.000  1.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.000  0.000  0.000  0.000  0.0  0.0  0.0  0.0  0.0
```

Kinetic Constants for Leach Reactions :

```
.3000E-02 .7621E-04 .1580E-05 .1215E+04 .8501E+02 .2036E+03 .1169E+03 .0000E+00 .0000E+00 .0000E+00
.0000E+00 .0000E+00
```

Stoichiometric Constants for CIP Reactions :

```
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0 -1.0 -1.0 -1.0 -1.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 -0.5  0.0  0.0
-1.0 -1.0 -1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0 -1.0 -1.0 -1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0 -1.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
```

Kinetic Constants for CIP Reactions :

```
.4393E-03 .2196E-03 .4393E-03 .9000E-04 .4500E-04 .9000E-04 .2000E-04 .1000E-04 .2000E-04 .1300E-04
.2300E-07 .0000E+00
```

I.6 PHYS.DAT : PHYSICAL CONSTANTS DATA FILE

μ	ρ
18.015	1.000
60.085	2.650
74.094	2.430

40.080	0.000
17.007	0.000
26.018	0.000
31.998	0.000
196.967	19.300
196.967	19.300
249.003	0.000
63.546	8.950
63.546	8.950
115.582	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
18.015	1.000
60.085	2.650
26.018	0.000
31.998	0.000
249.003	0.000
115.582	0.000
12.011	1.400
12.011	1.400
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000
0.000	0.000