

A Population Balance Approach to the Modelling of the CIP Process

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A method, based on the macroscopic population balance equation allowing the dynamic simulation of a multistage adsorption plant given an arbitrary rate expression, is described. The partial differential equations resulting from this method are simplified using the method of characteristics. The simplified equations can then be solved using standard ODE integration techniques. The procedure is illustrated by means of data typical of a CIP application.

Requirements for data structures which allow the incorporation of the carbon-in-pulp (CIP) model (and other unit models) into a general metallurgical simulator are described. Based on these considerations, it is concluded that more generality in the description of distributed quantities such as loading and particle size is provided by the use of mass density at fixed class boundaries, rather than discrete masses within fixed classes as has hitherto been used by ore-dressing simulators.

Introduction

A number of metallurgical simulation packages exist although many of these are not general simulation packages which allow the simulation of arbitrary process flowsheets. Packages which allow the simulation of arbitrarily complex ore-dressing flowsheets have been described, (1) and some packages which permit the simulation of ore-dressing and hydro-metallurgical flowsheets using simplistic models are also available. (2)

Cilliers (11) has developed a flexible simulator executive incorporating data structures which are extendable and versatile enough to describe all possible substream types found in hydro-metallurgical flowsheets. Powerful tearing and ordering routines which are able to cope with the complex recycles present in these flowsheets were also developed. (11) Although some excellent work in the modelling of particular hydrometallurgical

unit processes has been done, (12) no common methodology such as that used for ore-dressing modelling exists.

This paper describes the modelling of the CIP process. The techniques developed to model this process may serve to illustrate some methods which may be used in the modelling of hydrometallurgical processes such that the resulting models can be used in a general simulator.

Owing to the economic importance of the CIP process in South Africa as well as in other gold producing countries, the benefits which an accurate, flexible model could have for the design and optimization of CIP plants are obvious. This is one reason why a CIP modelling exercise was chosen. The other is that the CIP process is complex and any methods developed for its modelling are likely to have significant implications for the development of simulation techniques for

hydrometallurgical unit processes. This would facilitate the development of a simulator which is able to handle metallurgical flowsheets containing both ore-dressing and hydrometallurgical unit processes.

Ore-dressing simulator data structures

The success realized by available ore-dressing simulators is perhaps due to the more simplistic models of unit processes (as compared to, say, hydro-metallurgy) with which they have to contend. There is also only the ore phase which needs to be described effectively. In general, only the mass flowrate of the aqueous phase is needed. This has allowed the development of data structures which represent the properties of the process streams in great detail. For ore-dressing, attention has focused on the description of the particulate nature of the ore. In the well known ore-dressing simulator MODSIM, (1) a three dimensional matrix represents the distributed properties of particle size, grade and 'floatability' as a discrete distribution for each process stream. Each mathematical model in the simulator thus operates on a well defined stream data structure, transforming the discrete feed distribution into the appropriate distributions for the unit products. Calculation may then proceed easily in sequential-modular fashion.

Considerable success has been obtained using this method, and as most ore-dressing models described in the literature use this discrete method for representing the distributed ore properties, it is easy to add new unit process models to such a simulator.

The development of techniques for the modelling of the CIP process

Although significant research has been conducted on the derivation of an

appropriate rate expression for the adsorption of gold onto activated carbon, (3,4,5) not much work concerning the insertion of these rate expressions into the equipment mass-balance has been done. It is normal to develop particular methods appropriate for the rate expression used. (4,5) This is obviously unsatisfactory if the models developed are to be embedded in a general simulator. The CIP model should be capable of accepting a user-supplied rate expression. The level of complexity (in the rate expression) may thus be chosen to suit the amount and type of data to which the user has access.

Quantities which have a major effect on the rate of adsorption of gold onto carbon are bulk solution tenor, carbon particle size and gold loading on the carbon. Each rate expression includes these variables (or closely related quantities) in a specific functional form to predict the rate of loading at any time. Due to the nature of the carbon used in CIP plants and the way in which it is manufactured, the carbon particles are not equally sized but a distribution of sizes exists. Carbon is transferred countercurrent to the flow of the pulp by moving a certain fraction of the carbon in each contactor forward to the next contactor periodically. This leads to a distribution of loadings (which can be expected to be different for each particle size) in each contactor. Thus two distributed quantities exist which strongly influence the rate of adsorption. These must be dealt with appropriately in any attempt to model the CIP situation.

Williams and Glasser (5) have shown that if the rate expression is linear in the gold loading term, average loading values may be used in both the carbon mass balance and the solution mass balance. Van Deventer (4) used a discrete density function to describe the distribution of loadings. Although good agreement between

predicted and experimental data was obtained, it would be difficult to use this method to simulate the general case i.e. when carbon flows into and out of the contactor and carbon abrasion and breakage takes place during adsorption.

Due to the power and flexibility of the method, this work was based on the population balance technique.

The population balance technique

The population balance technique is a general method used to analyse particulate systems. It has been used to model crystallizers (6) as well as minerals processing unit operations such as comminution, (8) flotation, (10) and leaching. (7) Various examples of the use of population balance models in minerals processing are provided by Herbst. (9)

Although excellent explanations of the derivation of the population balance equation can be found in the above references, a short review is in order for those readers not familiar with the relevant literature.

Although derived from the same mathematical equations, two forms of the population balance exist: the macroscopic and microscopic forms. The macroscopic version is used when the behaviour of each particle is not influenced by its position in the reactor vessel. This form is normally used for systems where it can be assumed that the particulate phase is well mixed, such as leaching and CIP. The microscopic form is used to describe systems where the particle behaviour is influenced by its spatial coordinates, for example in a plug-flow reactor. Only the macroscopic population balance equation will be discussed in this paper as it is assumed that the carbon phase in an adsorption vessel is well mixed.

A particle is considered to have a set of properties $Z_1, Z_2 \dots Z_J$. These may

be properties such as particle size, unreacted core size (shrinking core leaching model), the number of radicals in a polymer, or the loading of gold on a carbon particle. The continuous rate of change of each property is defined by $\nu_i = dZ_i/dt$.

$\Psi(Z_1, Z_2, \dots Z_J)$ is a population density function defined so that $\Psi(Z_1, Z_2, \dots Z_J) dZ_1 dZ_2 \dots dZ_J$ represents the number of particles per unit volume, which have property 1 in the range Z_1 to $Z_1 + \Delta Z_1$, property 2 in the range Z_2 to $Z_2 + \Delta Z_2$ and so on.

A number balance (9) then leads to the macroscopic population balance equation :

$$\frac{\partial [V(t)\Psi]}{\partial t} = \sum_{i=1}^{\text{feeds}} F_i^{\text{in}} \Psi_i^{\text{in}} - \sum_{i=1}^{\text{products}} F_i^{\text{out}} \Psi_i^{\text{out}} + V(t) \left[(B-D) - \sum_{j=1}^J \frac{\partial (\nu_j \Psi)}{\partial Z_j} \right] \quad [1]$$

For the CIP case the distributed quantities are loading y and particle size δ . Thus define $\Psi(y, \delta, t) dy d\delta$ as the number of particles having loading between y and $y + \Delta y$ and particle size between δ and $\delta + \Delta \delta$ at time t , per unit volume of carbon in the contactor. The property velocities are thus :

$$\nu_1 = \frac{dy}{dt} = R(y, C, \delta)$$

$$\nu_2 = \frac{d\delta}{dt}$$

The following conditions are assumed to exist during an adsorption cycle :

- No carbon flows into or out of any of the contactors.

$$\Rightarrow F_{\text{in}} = F_{\text{out}} = 0$$

$$\Rightarrow V(t) = \text{Constant}$$

- No breakage or attrition of carbon occurs.

$$\Rightarrow B = D = 0$$

$$\Rightarrow d\delta/dt = 0 = \nu_2$$

The first assumption is restrictive in that, in general carbon may flow into or out of a contactor owing to screen leaks, spills or carbon transfer. This may be accommodated easily in the macroscopic equation. In this paper the simple case will be developed so as not to make the development more complex than necessary. The first assumption is thus not a limitation of the method but is used merely for convenience in this particular case. It can be seen that if functional forms for ν_2 , B and D exist, then the macroscopic equation could be used to model the industrial-scale adsorption process realistically i.e. for the case where carbon abrasion and breakage as well as carbon flow into and out of a contactor takes place.

Equation [1] for the assumptions made can thus be written for each adsorption stage n as :

$$\frac{\partial \Psi_n}{\partial t} + \frac{\partial}{\partial y} \left[R(y, C_n, \delta) \Psi_n \right] = 0 \quad [2]$$

with $\Psi_n(y, \delta, t_0) = \Psi_{n,o}(y, \delta)$.

As it has been assumed that no size degradation occurs, it is possible to substitute the more convenient mass density P_n for Ψ_n . $P_n(y, \delta, t) dy d\delta$ is thus the mass of carbon in the contactor having loading between y and $y+\Delta y$ and size between δ and $\delta+\Delta\delta$ at time t . It is easily shown that [2] can be written as :

$$\frac{\partial P_n}{\partial t} + \frac{\partial}{\partial y} \left[R(y, C_n, \delta) P_n \right] = 0 \quad [3]$$

with $P_n(y, \delta, t_0) = P_{n,o}(y, \delta)$.

Equation [3] is a first-order PDE which

describes the movement of the carbon loading and size distribution function in each stage with time. This equation must be solved simultaneously with the liquid mass balance which can be written as follows (assuming perfect mixing, and that no leaching takes place) :

$$\frac{dC_n}{dt} = \frac{Q}{V_s} (C_{n-1} - C_n) - \frac{1}{V_s} \int_0^\infty \int_0^\infty P_n(y, \delta, t) R(y, C_n, \delta) dy d\delta \quad [4]$$

with $C_n(t_0) = C_{n,o}$

The Equations [3] and [4] define completely the dynamic behaviour of a CIP plant subject to the assumptions stated above.

Methods of solution

The system of Equations [3] and [4] can be simplified using the method of characteristics. (13) This method finds directions in the relevant plane(s) which transforms the integration of a system of PDEs into the integration of a system of ODEs. Suitable methods for integrating ODEs can then be applied, preferably algorithms which adjust the step size to keep the error below a maximum bound such as that described by Fehlberg. (14)

Applying the method of characteristics to the system of Equations [3] and [4], the characteristic directions are given by :

$$\left. \frac{dy}{dt} \right|_I = R(y, C_n, \delta) \quad [5]$$

$$\left. \frac{dy}{dt} \right|_{II} = 0 \quad [6]$$

Along these directions the equations to be integrated are :

$$\left. \frac{dP_n}{dt} \right|_I = - P_n \frac{\partial R(y, C_n, \delta)}{\partial y} \quad [7]$$

$$\left. \frac{dC}{dt} \right|_{II} = \frac{Q}{V_s} (C_{n-1} - C_n) - \frac{1}{V_s} \int_0^{\infty} \int_0^{\infty} P_n(y, \delta, t) R(y, C_n, \delta) dy d\delta \quad [8]$$

The system of equations to be solved are thus [5], [7], [8] with the appropriate initial conditions.

Carbon streams data structures suitable for use in a general simulator

Any general simulator must be able to represent distributed properties in such a way that the data for all streams is 'indexed' by the same fixed class boundaries. For example, in an ore-dressing simulator such as MODSIM, the contents of size class 3, in any stream, may refer to the mass of particles in that stream having a representative size of 300 μm . The models transform the contents of these classes, but do not change the 'index' values of any classes.

When transferring carbon in a CIP plant, a mixing operation is carried out, with a fraction of the carbon in two adjacent stages being mixed together. In order to facilitate the simulation of this mixing operation, the distributed properties (loading, size) of the carbon in each stage must be indexed by the same fixed class boundaries. Thus loading class 4, size class 3 in contactors 1..N must all represent the mass or number density of carbon in each contactor having say loading 300 g/ton and particle size 1.5mm. This is even more important if the flowsheet to be simulated contains other carbon handling units, for example an elution column, or the more complex CIP case where flow of carbon into and out of the contactor (owing to carbon transfer and/or spills) is modelled.

The elution and CIP mathematical models are then able to operate on the streams

data using a common 'index' which needs to be stored only once for the entire flowsheet, and not for each stream. Considering the number of classes which may be needed to obtain an accurate simulation, this obviously leads to significant savings in memory requirements.

There are two possible methods for implementing fixed class stream storage for the particulate phase. One is to use discrete masses at fixed representative class values by discretizing the population balance partial differential equation. A good example of this is the way in which the PDE arising from the breakage and selection comminution model is discretized. Ore-dressing simulators such as MODSIM then store the actual mass in each class in each stream. However, for certain models such as the CIP model (see Equation [1]) it may be necessary to approximate a partial derivative using finite differences if the PDE is to be discretised. Finite difference methods are not suitable if discontinuities exist in the density function, (15) and discontinuities may easily occur in the initial conditions for the population balance Equation [1]. These methods do not propagate the discontinuity, but "smudge" the area near the discontinuity.

The other method is to use mass or number density at fixed class bounds. Sepulveda (7) has used this method in the numerical techniques that he has developed to solve rigid models for the leaching process.

The approach adopted in this work was to use mass density at fixed class bounds. This was done for the following reasons :

- a) The method of characteristics can then be used to solve the CIP model with any rate expression. This can be seen from Equations [5], [7] and [8]. This method can be used for rate expressions

of any complexity, even when a system of differential equations such as those developed by Van Deventer (4) describe the rate of adsorption. A sophisticated ODE solver has been designed, and this forms the basis of the CIP model. This solver is based on the work by Fehlberg (14) which allows an estimate of the truncation error to be made at each integration step. Step length control is implemented using methods recommended by Thomas (17). This ODE solver allows the solution of all the differential equations defining the rate expression as well as the characteristic equations.

- b) Sufficient generality is provided. The model can be extended to cope with the general CIP case (where carbon may flow into and out of a contactor) and still use any rate expression.
- c) The population balance method is powerful enough to provide the framework for the modelling of many other unit processes. These models would require the distribution to be described as discrete masses or mass densities, and as it may not always be possible to discretize the population balance PDE, the use of mass density provides more generality. Mass or number density thus provides a common basis for future model development, enabling program modules and methods to be developed which can be utilized by all unit models.

Implementation using the method of characteristics

Using characteristics, the problem consists of integrating Equation [5] for the chosen number of characteristics. The number of characteristics used depends on the accuracy required. Ten to two hundred characteristics per contactor were used, and it was found that forty

characteristics per contactor provided acceptable accuracy for the case simulated. The number of characteristics chosen determines the number of equations to be solved. Although microcomputers provide sufficient storage capability even when two hundred characteristics are used, the numeric processing capabilities of most microcomputers are such that times in the order of hours would be needed to solve the large system of ODEs which define this problem. This is made worse by the fact that the system may need to be solved many times, starting at some initial condition, before a pseudo-steady state is achieved. This makes the use of (most) microcomputers to solve the problem impractical at this stage.

The initial value for each characteristic is the relevant fixed class boundary value. The characteristics define the trajectory of a particle which has an initial loading equal to a class boundary value. Equation [8] needs to be integrated along each characteristic, with the initial conditions being the initial number density at the appropriate class boundary. Equation [7] also needs to be integrated simultaneously with [5] and [8]. As the y values defined by the integration of [5] are not equally spaced the trapezoidal rule was used to evaluate the integral in [7].

The major problem resulting from the use of characteristics is that at the end of the adsorption cycle, P is defined at the y values calculated by the integration of [5], not at the fixed class boundaries. An interpolation procedure was thus developed which enabled the values of P at the fixed class bounds to be found from the values of P defined by [5] and [8] at the end of the adsorption cycle.

An appropriate interpolation technique

The requirement for the interpolation technique was that the integral :

$$I = \iint P(y, \delta, t) dy d\delta$$

evaluated at the y, δ, P values defined by the integration of Equations [5] and [8], be the same as that evaluated at the fixed class bounds. This is most critical as the above integral is the total mass of particles in the contactor at time t and this quantity cannot be in error.

Although standard linear and polynomial interpolation techniques were tried, none met the above requirement. Accordingly, a method based on constrained minimization was developed. The constraint in the interpolation method developed is that the integral calculated at the fixed class bounds be equal to I i.e. the total mass of carbon in the contactor. The quantity to be minimized is the sum of the relative differences between the P values at the fixed class bounds that satisfy the constraint and those P values determined

at the fixed boundaries by linear interpolation from the values defined by integration along the characteristics. This allows the constraint to be met while preserving the shape of the P distribution. A set of equations in P at the fixed class bounds is set up. These may be solved simply without using any complex numerical techniques. Figure 1 shows an example of results obtained using this method.

Simulation results

Although many simulations could be run showing the effect of various parameters on CIP plant performance, this work is primarily concerned with the description of changes in the loading distribution during adsorption. Thus only examples illustrating this feature will be presented.

All simulations were performed using

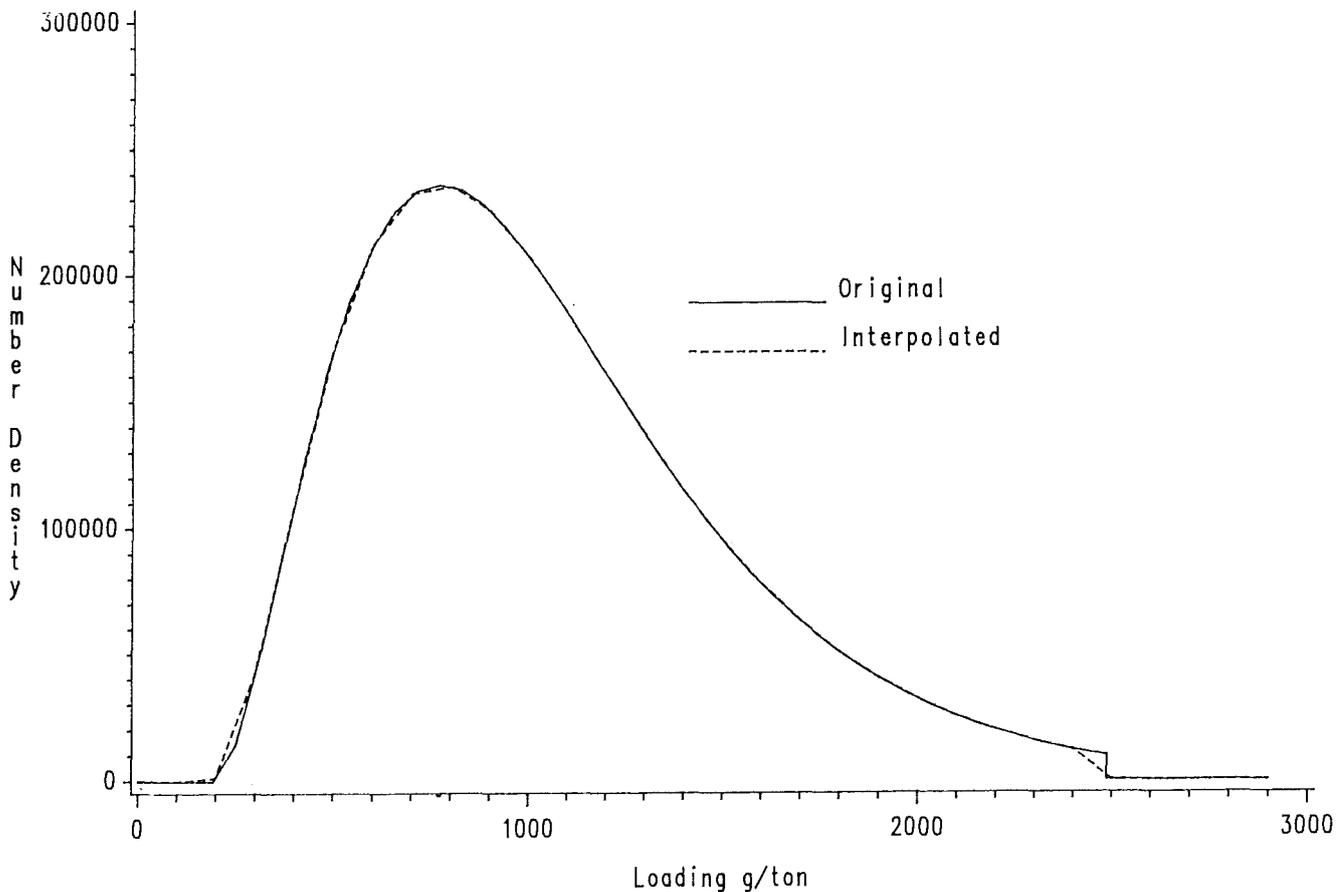


FIGURE 1. Original and interpolated distributions

the rate expression described by Menne (16) and used by Glasser and Williams (5) in their work. As the dependency of the rate expression parameters on carbon particle size have not been established, only one size class was used in all simulations. The following parameter values were used :

- $k_1 = 0,012$
- $k_2 = 0,0019$
- $y^* = 3328 \text{ g ton}^{-1}$
- $M_c = 4,32 \text{ tons}$
- $V_s = 75 \text{ m}^3$
- $Q = 75 \text{ m}^3 \text{ hour}^{-1}$
- $N = 5$
- $C^{in} = 1,9 \text{ g m}^{-3}$
- Cycle Time = 24 hours

The rate expression used has the functional form :

$$R = k_1 C (y^* - y) - k_2 y$$

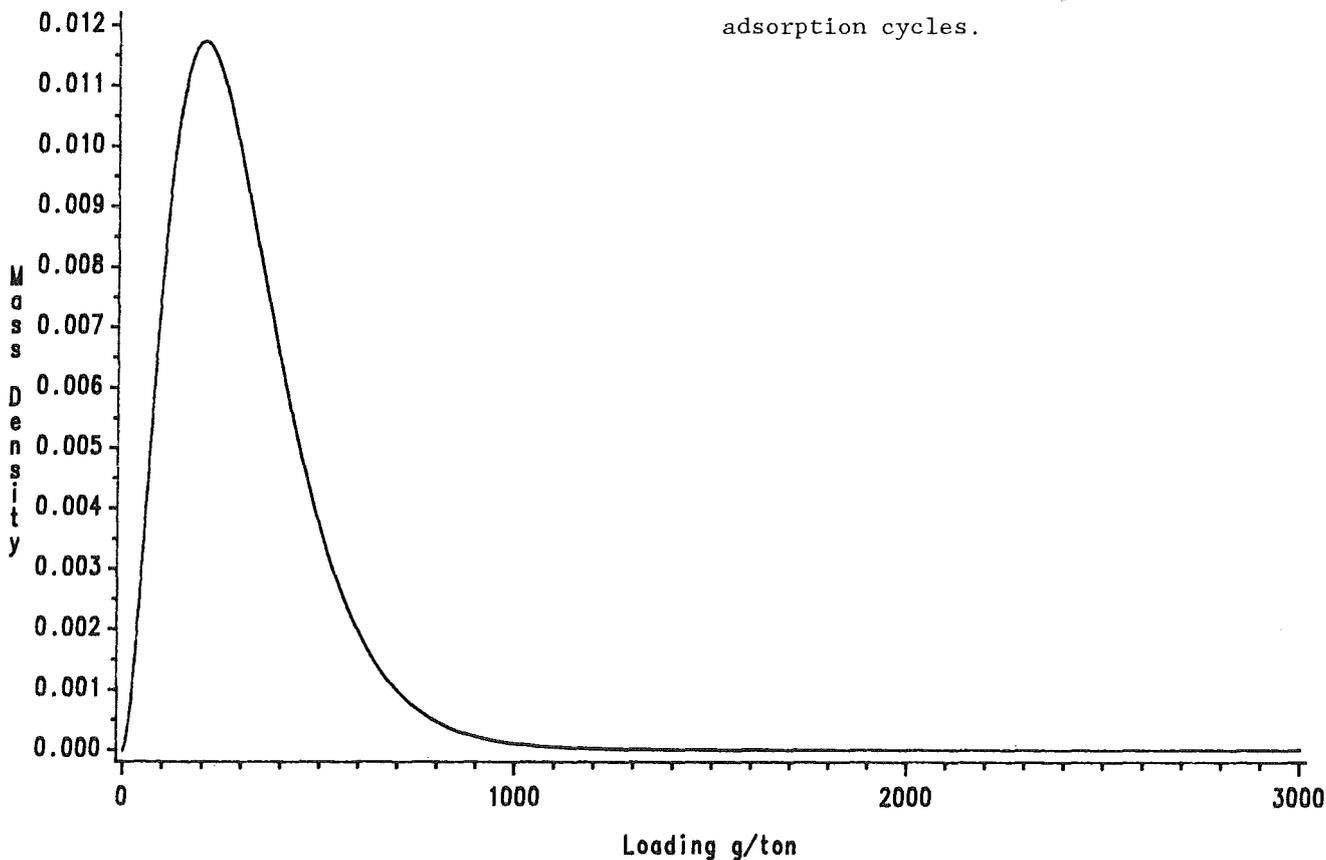


FIGURE 2. Initial density distribution in all CIP contactors

Figure 2 illustrates the distribution used as initial conditions in all CIP contactors.

Figures 3,4 and 5 illustrate how the loading distribution changes as the system converges to a pseudo steady-state. For this example 50% of the carbon in each stage was moved forward to the next stage after each adsorption cycle, the length of each cycle being 24 hours.

Figure 6 is a 3-dimensional plot showing the movement of the loading density distribution in stage 1 with progressive adsorption cycles.

Figures 3,4,5 and 6 all show the loading distribution after carbon has been transferred at the end of the relevant adsorption cycle. Figure 7 illustrates the effect of mixing carbon from stage 2 into stage 1 on the loading distribution in stage 1 after one adsorption cycle.

Figure 8 illustrates how the amount of carbon transferred affects the loading distribution in stage 1 after 15 adsorption cycles.

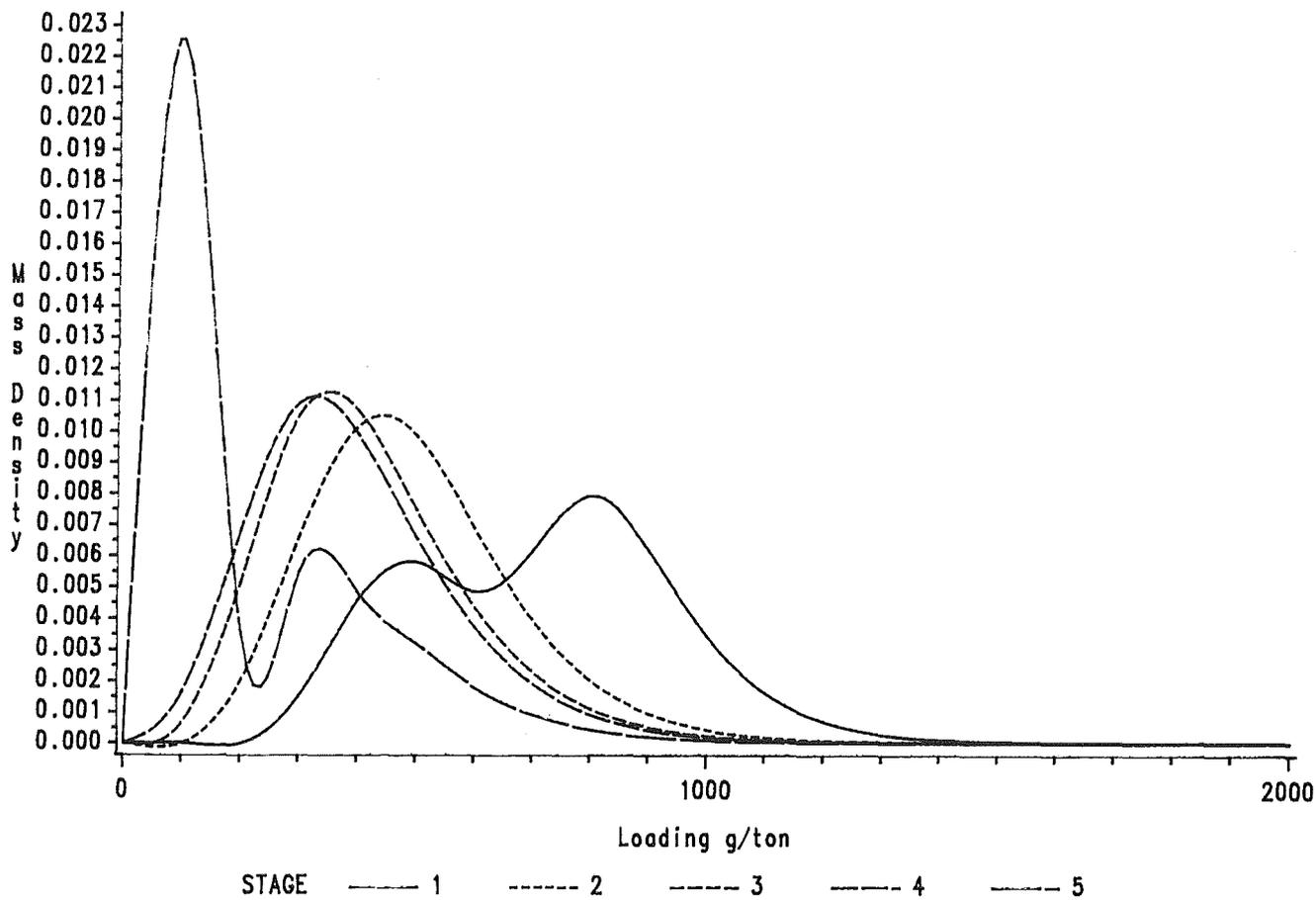


FIGURE 3. Distributions after 1 adsorption cycle

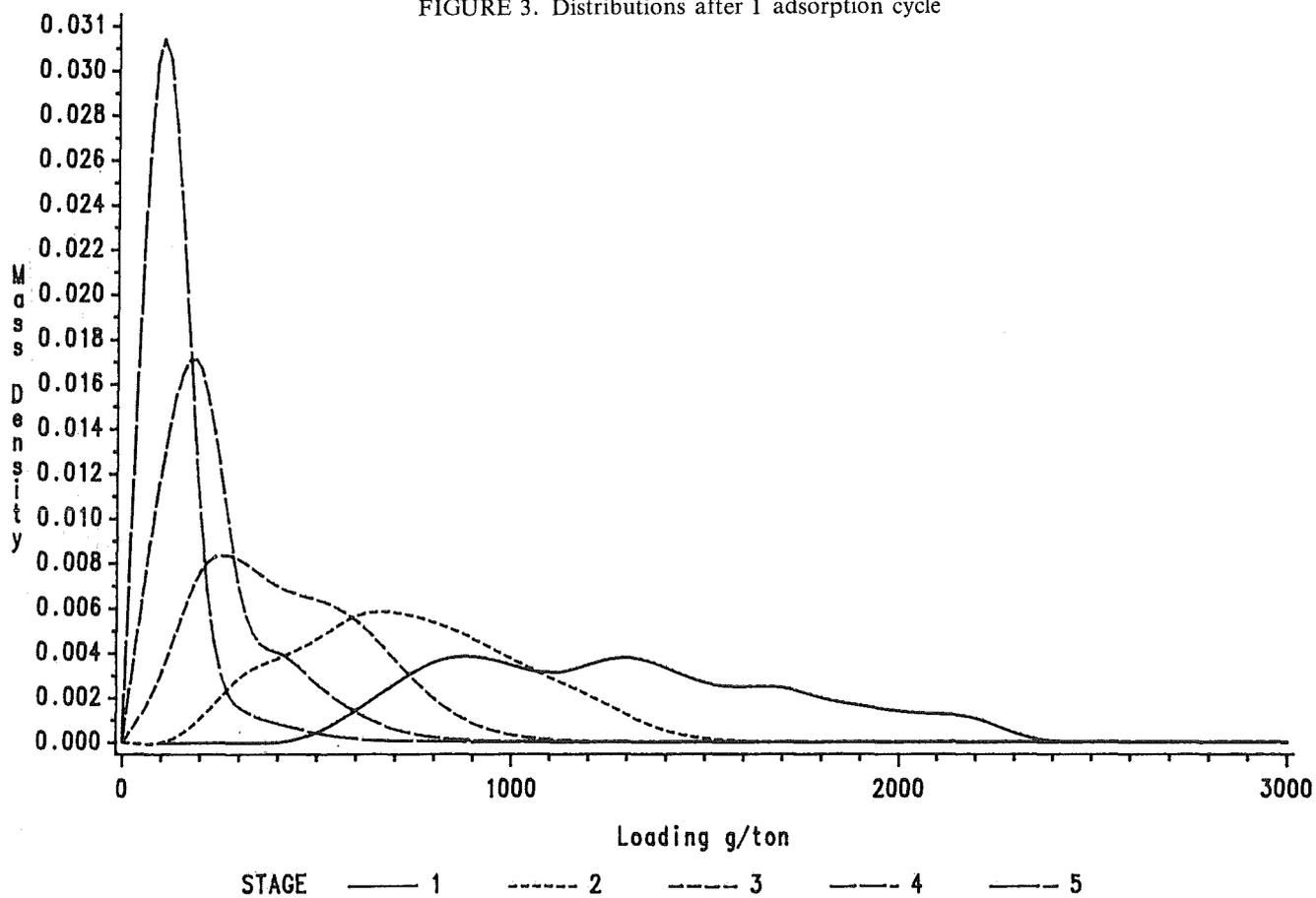


FIGURE 4. Distributions after 5 adsorption cycles

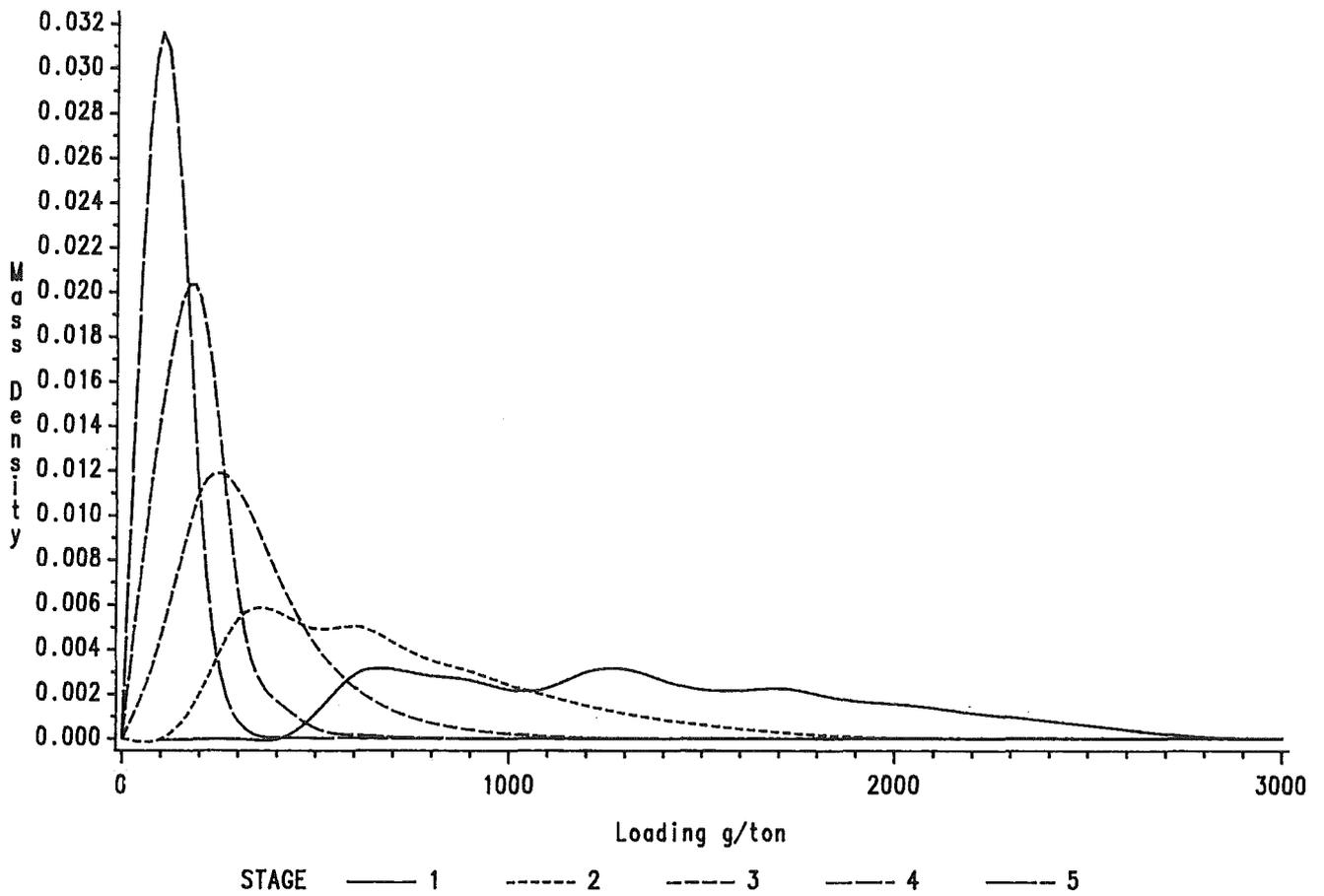


FIGURE 5. Distributions after 10 adsorption cycles

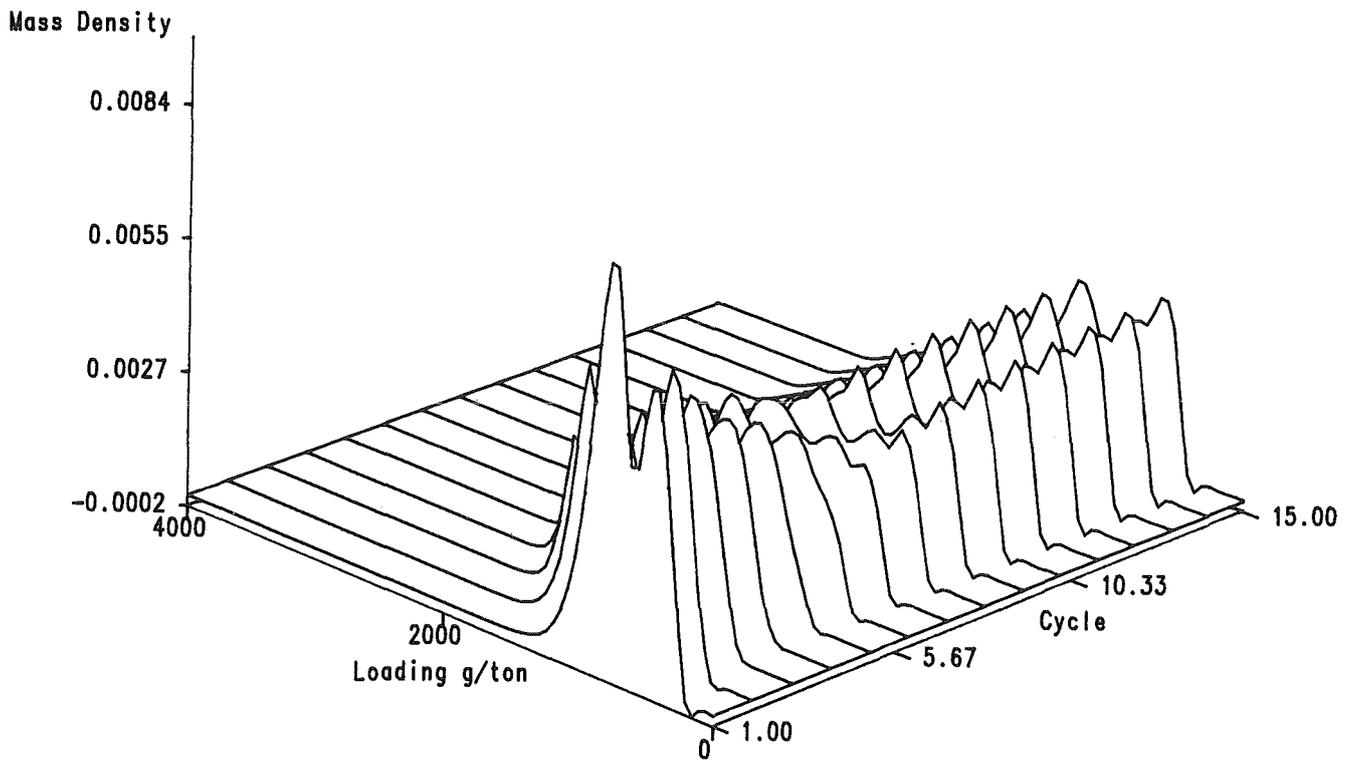


FIGURE 6. Movement of loading distribution in stage 1 as steady-state approaches

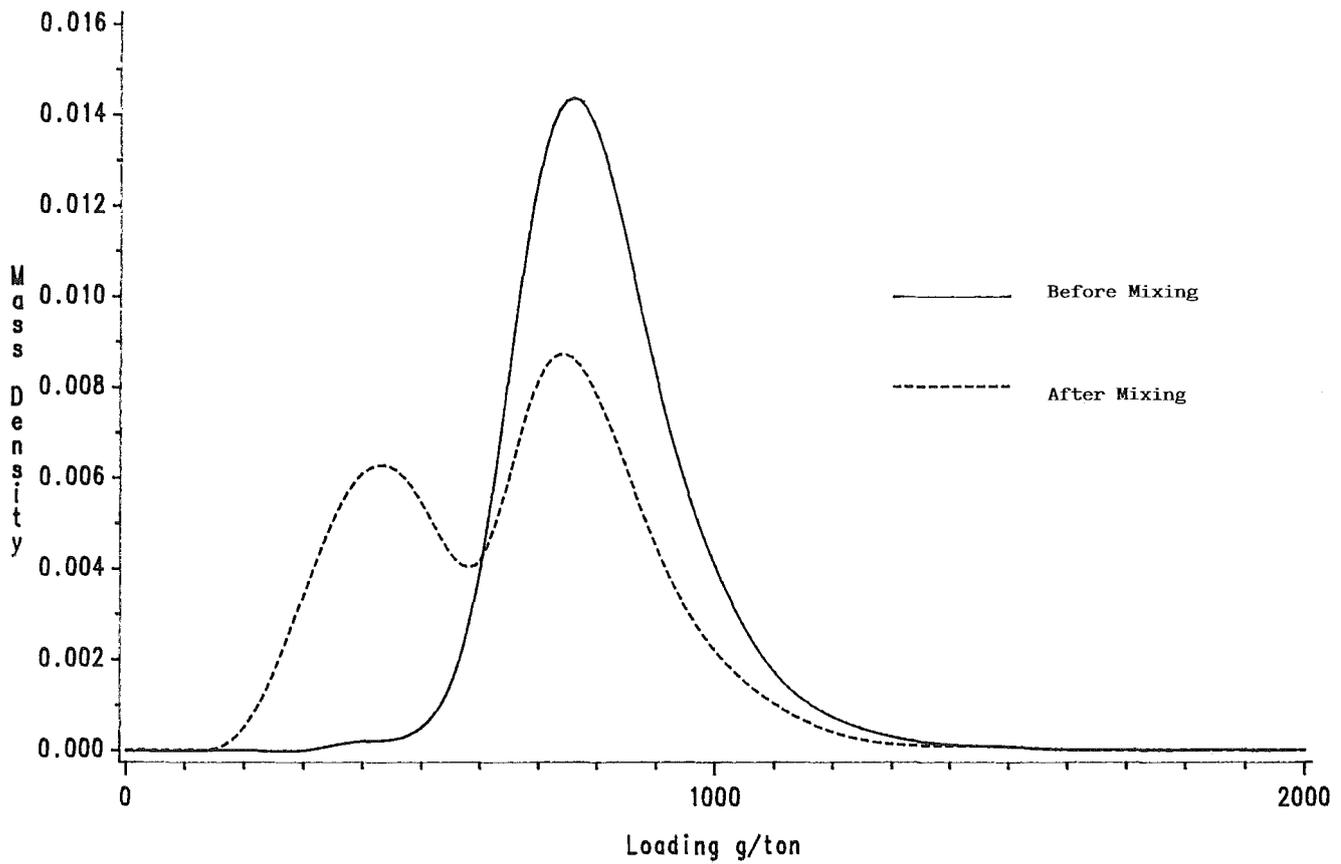


FIGURE 7. Results of mixed carbon from stage 1 and stage 2 after 1 adsorption cycle

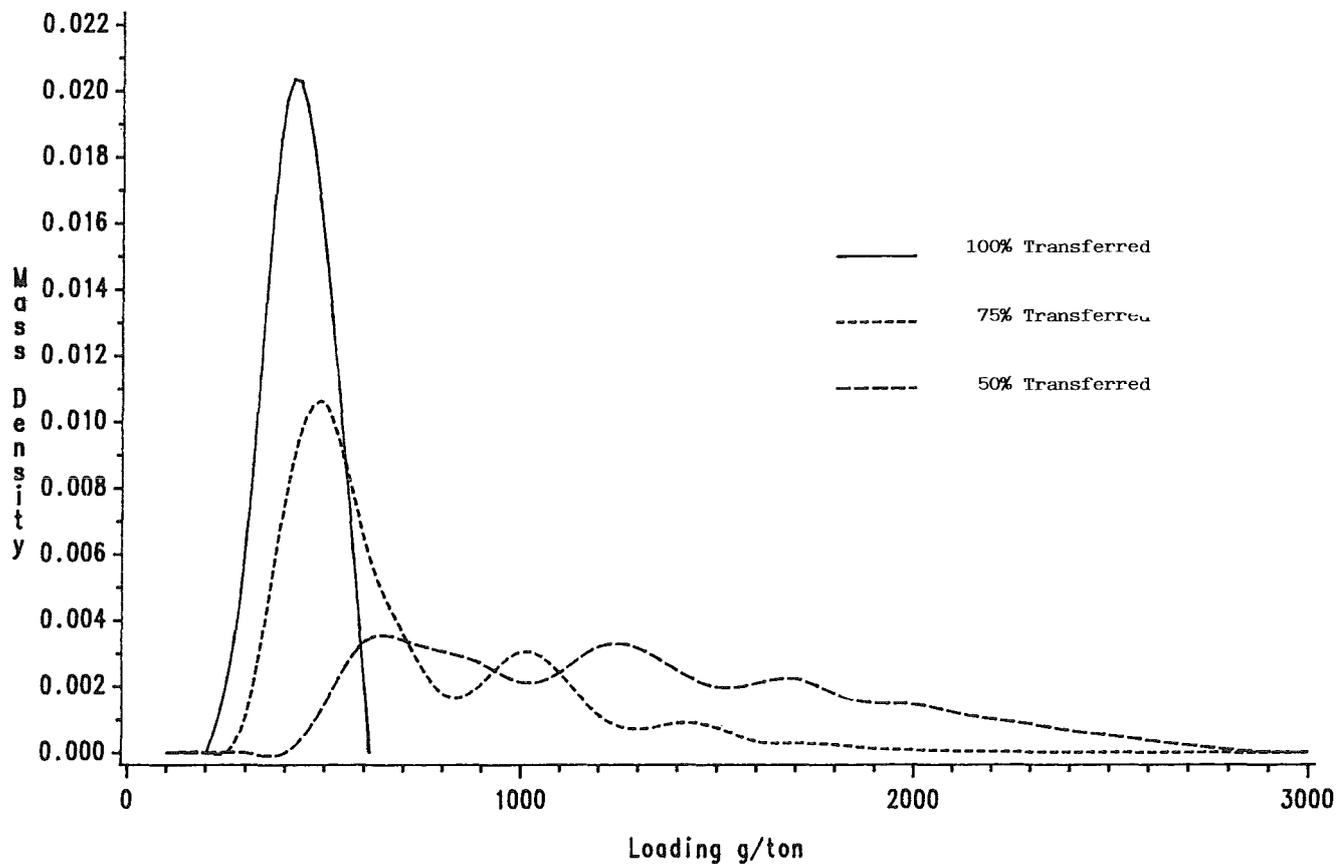


FIGURE 8. Effect of amount of carbon transferred from each stage after 15 adsorption cycles

Conclusions

A powerful technique, allowing the dynamic simulation of a CIP plant using any rate expression has been developed. This makes the simulation of RIP (resin in pulp) simple if an appropriate rate expression for the adsorption of gold onto resin is available, as the RIP equipment geometry is very similar to that of CIP.

The mass balance for the carbon phase was derived using the macroscopic population balance. The resulting system of equations was simplified by use of the method of characteristics and solved by conventional ODE numerical techniques.

Fixed class boundaries, together with mass density were used for the representation of the distributed carbon properties instead of the more commonly used discrete masses in fixed classes. This was done to provide maximum model generality and extendability.

The methods developed may be used as a basis for the development of other dynamic hydrometallurgical models, particularly other units which are found in resin or carbon based adsorption flowsheets such as elution.

Notation

- Ψ = Number density function.
 P = Mass density function.
 B = Birth rate function.
 D = Death rate function.
 V = Volume of particulate phase.
 M_c = Mass of carbon in a contactor.
 V_s = Solution volume in a contactor.
 F = Volumetric flowrate of particulate phase.
 Q = Volumetric flowrate of aqueous phase.
 N = Number of CIP stages.
 y = Average gold loading on carbon particle.
 d = Carbon particle size.
 C = Gold concentration in aqueous phase.

R = Rate of loading of gold onto a carbon particle.

Subscripts

n = Stage index.

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