Mathematical Modelling : A Wonderful Tool If Judiciously Used

(Lecture delivered on 21st August 2003)

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Professor Surya Pratap Mehrotra Director, National Metallurgical Laboratory, Jamshedpur was born on 26th April, 1947 in Kashipur (Dist. Udham Singh Nagar), Uttaranchal. He did his BTech (1968), MTech (1970) and PhD (1973) in Metallurgical Engineering from IIT, Kanpur. He has been a Professor in the Department of Materials and Metallurgical Engineering and Dean of Faculty Affairs, Indian Institute of Technology (IIT), Kanpur before taking the present assignment.

Prof. Mehrotra has extensively travelled abroad on Academic assignments. He was a Visiting Professor at the University of British Columbia, Vancouver, Canada during 1979-81, Visiting Scientist during 1983-85. He was at the Pennsylvania State University at University Park during 1987 as a part of the Indo-US Science of Technology Initiative. He has visited several other Universities like University of California at Berkeley, Carnegie Mellan University, Columbia University, M.I.T., Purdue University, University of Pittsburg in U.S.A., McGill, Montreal and Toronto Universities in Canada, Imperial College and Sheffield University, in U.K. He has been to LuleaSweden, Maastrich-Netherlands, Florence-Italy and Montreal-Canada for participating in various International Conferences.

Professor Mehrotra is a renowned Process Metallurgist and one of the pioneers in this country to take up Mathematical Modeling and Simulation of Mineral and Metallurgical processes. He has a wide spectrum of research interests ranging from Mineral Processing to Materials Science. Some of his pioneering research contributions include: Mathematical modeling of froth flotation Kinetics; Synthesis and optimal design of flotation circuits; Settling behaviour of particles in jigs; Studies on hydrodynamics in Pachuca tanks used for leaching of Uranium, Zinc and Gold ores; Mixing phenomena in gas agitated liquid baths; Studies on magnetohydrodynamics in Hall-Heroult cells used in production of aluminium; Near net shape casting of metal and composite sheets using simple roll continuous sheet caster; Kinetics of gas solid reactions in fluidized bed reactors; Prediction of thermal behaviour to predict freezeline in the subhearth of an iron blast furnace and Prediction of surface energies in metal-ceramic systems. The uniqueness of his researches is that most of his modeling and simulation investigations have been accompanied by judiciously designed, rigorous experimental studies for data generation needed for validation of mathematical models.

As an outstanding teacher, Professor Mehrotra has designed and developed several new courses both at the graduate and undergraduate levels at IIT Kanpur and University of British Columbia, Vancouver, Canada. These include Mathematical Modeling of Metallurgical and Mineral Processes; Process Control in Metallurgy;

Metallurgical Kinetics; Unit Operations and Processes in Extractive Metallurgy; Science and Technology of Non-Ferrous Metal Extraction; Process Plant Design for Metallurgical Operations. He has guided 3 Ph.Ds, about 35 M. Techs. and a large number of BTech. projects.

Professor Mehrotra has been very enthusiastic in organising Continuing Education activities as well. He has developed and offered several courses/ programmes, specifically designed for engineers/scientists working in industries, R & D organisations and academic institutions. Courses like Mathematical Modeling of Metallurgical Processes, Continuous Casting of Steel, Science and Technology of Mineral Processing and Transport Phenomena in Metallurgy have been repeatedly offered on request from industries.

While at IIT Kanpur, Professor Mehrotra has been involved in planning of education and directing research, and held several important administrative positions. He was the Co-ordinator of Quality Improvement Programme and Convenor, Continuing Education Programme (1988-90). He headed Metallurgical Engineering Department (1990-93) and Advanced Centre of Materials Science (1992-93). He has also been a member of Board of Governors of IIT Kanpur (1996 & 1997).

Professor Mehrotra has over 90 research publications in reputed National and International Journals and edited several Books and Monographs. He has organised and participated in a number of conferences/seminars at national as well as international levels and delivered keynote lectures and chaired technical sessions. He has received several awards and recognitions including: National Metallurgists' Day, Best Metallurgist Award, Ministry of Steel and Mines, Govt. of India (1992); Maharashtra Govt. Award for Outstanding Research Contributions, Indian Society for Technical Education, New Delhi (1993); Fellow of Indian Institute of Metals (2000); Fellow of Indian National Academy of Engineering (2001); Distinguished Metallurgist Award, The Institution of Engineers (2002); and IIM SAIL Gold Medal (2002); Best Metallurgical and Materials Engineers Award of the Institution of Engineers; IIME Mineral Beneficiation Award 2002;elected Fellow of The National Academy of Sciences, India (2003).

Professor Mehrotra is a member of the Minerals, Metals and Materials Society (TMS) of AMIE, USA, life member of Indian Institute of Metals, Indian Society for Technical Education, Metal Research Society of India. He has also served as Vice President (1996-2000) and President (2000-02) of Indian Institute of Mineral Engineers. He is presently the member of Programme Advisory Committee in Engineering under Science and Engineering Research Council, DST, New Delhi; Member of Research Advisory Council of Jawaharlal Nehru Aluminium Research Development and Design Centre, Nagpur; Member of Editorial Advisory Board of Indian Institute of Metals and member of review boards of several other national and international journals.

The excerpts of the lecture delivered by Prof. S. P. Mehrotra

Good Afternoon! I am going to talk on the topic "Mathematical modelling : A wonder tool if judiciously used". It took me a while to properly phrase the title of my presentation today. I did not want to make it too specific to be confined to one particular kind of activity, at the same time I did not want to talk about things which do not belong to me; and also I did not want to talk about mathematical modelling in general. In fact, this particular lecture represents the philosophy of my research career over the last 30 years.

I start with two basic definitions in the context of this lecture. Mathematical modelling, as you all know, is representation of chemical or physical phenomena in a process by one or more mathematical equations along with the necessary initial and/or boundary conditions. The equations involved could be algebraic, ordinary differential and/or partial differential. In the context of mathematical modelling, simulation may be defined as the study of process behaviour with respect to operating variables and process parameters. We come across mathematical modelling in almost all facets of engineering whether it is R&D, process design or plant operations. For instance in R & D, we often study reactions and processes and try to determine the kinetic parameters and study the mechanism of reactions. In almost all cases, it is done through modelling and simulation. It is a different thing that sometimes we realise it but more often we do not. The use of simple Arrhenius equation to estimate the activation energy and then try to comment about the mechanism of reactions or the rate phenomena in process is nothing but modelling. Another thing that we often do is to study the effect of process parameters on the process behaviour. This can be done by performing experiments in the laboratory - by changing the input parameters, measuring the output parameters and then try to infer from that about the process behaviour. Many a time, performing experiments even on laboratory scale may be quite expensive, time consuming and even risky. Mathematical models, these days, are being used in all spheres of engineering - from research and development to plant operations - and even in business and economic studies. In research and development, these are being used for: (i) determining chemical kinetics, mechanisms and parameters from laboratory or pilot plant research data, (ii) exploring the effects of different operating conditions for optimization studies, and (iii) aiding in scale up calculations. In the area of design, mathematical models find applications in: (i) exploring sizing and arrangement of process

equipment for dynamic performances, (ii) studying the interactions of various parts of the process, (iii) evaluating alternate control strategies, and (iv) simulating start-up, shut down and emergency situations and procedures. In plant operations mathematical models are used in: (i) trouble shooting, control and processing problems, (ii) aiding in start-up, (iii) studying the effect of and the need of expansion (bottleneck removal) of projects and (iv) optimizing plant operation.

STEPS IN THE DEVELOPMENT OF A MATHEMATICAL MODEL

The various steps involved in the building of a mathematical model of a complex process have been described by Himmelblau and Bischoff[1], are

1. Formulation of the problem and establishment of objectives.
2. Preliminary inspection and classification of the process to break it down into sub-systems.
3. Preliminary determination of the relationship among the sub-systems.
4. Analysis of the variables and relationships to provide as simple and consistent a set as possible.
5. Mathematical modelling of relationships in terms of the variables and parameters.
6. Evaluation of how well the model represents the real process.
7. Application of the model - interpretation and comprehension of results.

Fig. 1 indicates the cyclic (iterative) nature of these steps.

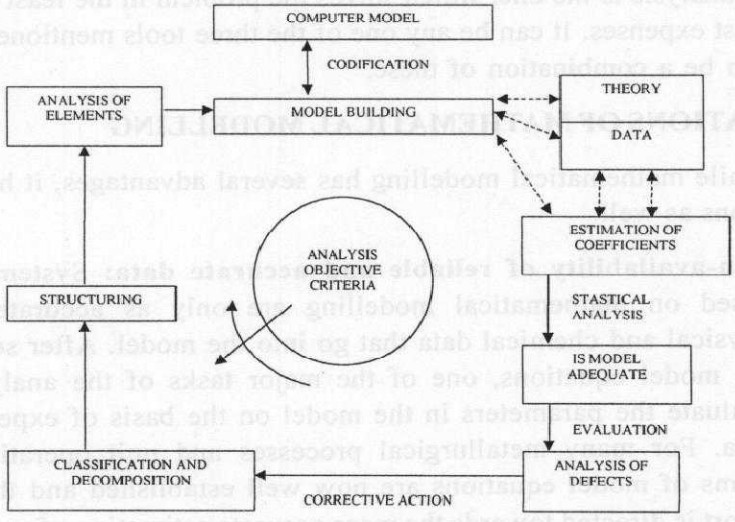


Fig 1. *Cyclic nature of steps in model building.*

Mathematical modelling is frequently hampered by a poor understanding of the process. This is more true for most metallurgical operations which often involve high temperatures and multiphase processes. In such situations, modelling must be undertaken hand-in-hand with sound experimental work. This point is vital to good model building and is emphasized throughout this lecture.

ROLE OF MATHEMATICAL MODELS IN PROCESS ANALYSIS

It is important that mathematical models be seen in correct perspective in Process Analysis. As an engineer, our principal objective is to know more and more about the process and its behaviour, i.e., how is it going to respond to changes under different input and operating conditions. This can be done by using one or more of the three commonly used tools. One, for an existing process we make measurements during its operation, compile data, analyse these as judiciously as we can and generate the kind of information needed. Second, generation of experimental data using replica or physical models of the operating units - real or simulated. The third tool, of course, is mathematical modelling. Thus it should be realised and emphasised that mathematical modelling is only one of the techniques or tools of process analysis - a very powerful tool, indeed. The point I am trying to emphasize is that mathematical modelling is not an end into itself and therefore, we should always remember as to what we are trying to do and why. And, of course, we should remember that the best method of process analysis is the one, which solves the problem in the least time and with least expenses. It can be any one of the three tools mentioned above, or it can be a combination of these.

LIMITATIONS OF MATHEMATICAL MODELLING

While mathematical modelling has several advantages, it has a few limitations as well:

1. **Non-availability of reliable and accurate data:** System studies based on mathematical modelling are only as accurate as the physical and chemical data that go into the model. After setting up the model equations, one of the major tasks of the analyst is to evaluate the parameters in the model on the basis of experimental data. For many metallurgical processes and unit operations, the forms of model equations are now well established and the entire effort is directed towards the more accurate estimation of parameters in these equations. Process kinetics is one area in which great

uncertainty exists. Normally, the kinetics coefficients are obtained by actually carrying out experiments in a small-scale reactor. Lack of information about side effects in small-scale reactors, effect of impurities in the actual commercial plant and improper scaling up criteria may lead to unpleasant surprises in the actual operation.

2. **Limitations in solving model equations** : Once the mathematical model is developed to describe the process, the equations involved in the model are to be solved using mathematical techniques. Most of the times, a process can be easily defined and described mathematically but the equations cannot be solved because of limitations in mathematical theories and computational techniques.

3. **Validity of assumptions** : The accuracy of the model depends on the validity of various assumptions. If the assumptions are too far off from reality, one cannot expect good results. So, while making certain assumptions to simplify a given set of equations, one should ensure that simplification does not turn into oversimplification.

4. **Extrapolation of a model** : Another danger in the use of model is to assume that the model represents the real system beyond the range of variables that the model was originally intended to encompass. Such extrapolation of the model may be very misleading. Fig. 2 illustrates an exaggerated case of extrapolation, by means of a linear model, into a region beyond the experimental data for a chemical reaction that reaches a maximum.

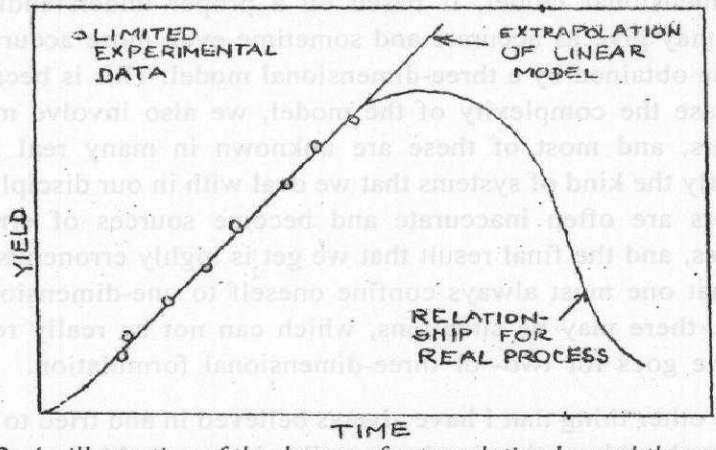


Fig 2. *An illustration of the danger of extrapolation beyond the range of variables.*

FALSE NOTIONS ABOUT MATHEMATICAL MODELLING AMONGST STUDENTS / YOUNG ENGINEERS

Many modellers start believing themselves to be intellectually more advanced as compared to their counterparts engaged in experimental activities. Often, the feeling is that while I can deal with complex mathematical formulations, they only do the experiments - a trivial job. Nothing can be more misleading than this. Another false notion that one often comes across is the belief that one can get complete information and solve all problems related to a process through a mathematical model. The truth is that most models are only ideal in nature and based on several assumptions. In fact, even the most sophisticated model would not be a true representation of a real process / phenomenon - it would only be an ideal representation since it is based on several assumptions. We must appreciate that the predictions we are making are only approximate and therefore, would give us only partial or incomplete information.

The other false belief is that a more rigorous or complicated model would give more accurate results. Contrary to it, many a times a well conceived but a very simple model can give quite reasonable results. I have seen students arguing 'Sir, you have only one-dimensional model, I have a three-dimensional model, then how do you say that your one-dimensional model may be adequate or even better than mine'. People who take several days to solve rigorous equations argue that their results are superior to those obtained by solving one-dimensional model equations in just few minutes or hours. Many a time, we find that even a one-dimensional model, if based on a proper understanding of the process, may give as accurate and sometime even more accurate results than those obtained by a three-dimensional model. This is because when we increase the complexity of the model, we also involve many more parameters, and most of these are unknown in many real situations, particularly the kind of systems that we deal with in our discipline. These parameters are often inaccurate and become sources of error, which propagates, and the final result that we get is highly erroneous. I am not saying that one must always confine oneself to one-dimensional model only. No, there may be situations, which can not be really represented unless one goes for two- or three-dimensional formulation.

One other thing that I have always believed in and tried to propagate is that one should use the simplest possible language. Many people during discussions tend to use very abstract and complicated terminologies,

which may have no bearing on the physics of the problem. My experience is that if a person repeatedly does it, it is because he is missing something some where. A good model formulation and its execution should be based on simple language, simple terminologies, and as I stated in the preceding paragraph, in many cases one need not go for the most rigorous formulation and solutions.

Many a times, the modellers think that experimental work has to be done by someone else. But, I strongly believe that the prerequisite for a researcher to be a good modeller is that he should be an equally good experimentalist. This, in fact, has been the philosophy of my R & D career throughout. In the remaining part of the talk I shall briefly discuss a few examples, all based on my own work. Except for the very first example, wherein the validation was done using actual plant data, in all other cases you would appreciate the kind of rigorous experimentation that was carried out, the data generated thereof and which then used to validate the model.

Example 1: Optimal Design and Synthesis of a Flotation Circuit[2]

Froth flotation is a mineral beneficiation process in which the valuable minerals are separated from their finely ground ores. The separation of valuable minerals by this process depends on the difference in the surface properties of the minerals involved. When a mixture of minerals is suspended in aerated water, the air bubbles tend to adhere preferentially to one of the constituents, which is more difficult to wet by water. In a single flotation cell there is one feed stream of raw ground ore slurry and two exit streams - the mineral rich floated 'concentrate' and the gangue rich 'tailings'.

Due to several reasons, the separation is seldom complete in a single flotation cell, and a number of interconnected flotation cells (or bank of cells) are used to improve the process efficiency. In a conventional flotation circuit, the feed is introduced in a 'rougher' cell, where a crude separation is affected. For improvement of the grade of the product, the concentrate is refloated in one or more 'cleaner' and 'recleaner' cells, and the tailings from the 'rougher' stage are refloated in 'scavenger' cells so as to extract more of the valuable residual mineral from the gangue rich stream. The issue under consideration is how to interconnect various flotation cells such that the separation efficiency of the flotation circuit is optimum. Since a typical flotation circuit may process several

thousands of tons of ore per year, even a marginal improvement in its process efficiency may have a significant economic impact. Hence, the optimal design and synthesis of large circuits is assuming importance. To understand the problem in this context, let me take a simple example.

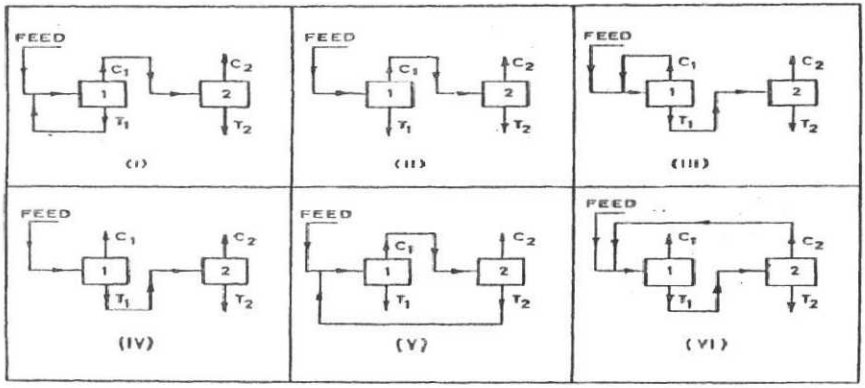


Fig 3. *Six possible configurations for a circuit with two flotation cells*

Suppose, I have to arrange two cells, what are the various possible configurations? How can I arrange these two cells, so that I get the best product? Six possible configurations are shown in Fig. 3. Instead of considering each individual circuit configuration, I can also consider a generalised circuit, Fig. 4, which embeds in it all possible configurations. This generalised configuration has one more major advantage that it has provision for recycling, withdrawal and feeding of partial streams.

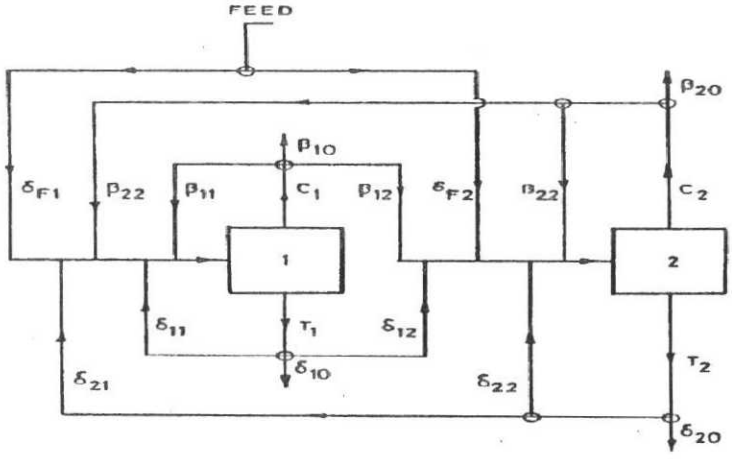


Fig 4. *Generalized configuration for two flotation cells.*

In actual practice, we have three or larger number of cells. A generalised circuit with four cells is shown in Fig. 5. Though it appears quite complicated, it contains in it the optimum circuit configuration as well. I now ask a question - can I evolve a methodology based on sound theoretical considerations to extract the optimum configuration for the given input conditions (i.e. type of material to be benificiated and other operating conditions) from this generalised circuit configuration? Without going into the details of mathematical formulation and analysis procedures, let me just briefly talk about the concept involved in the methodology developed by us.

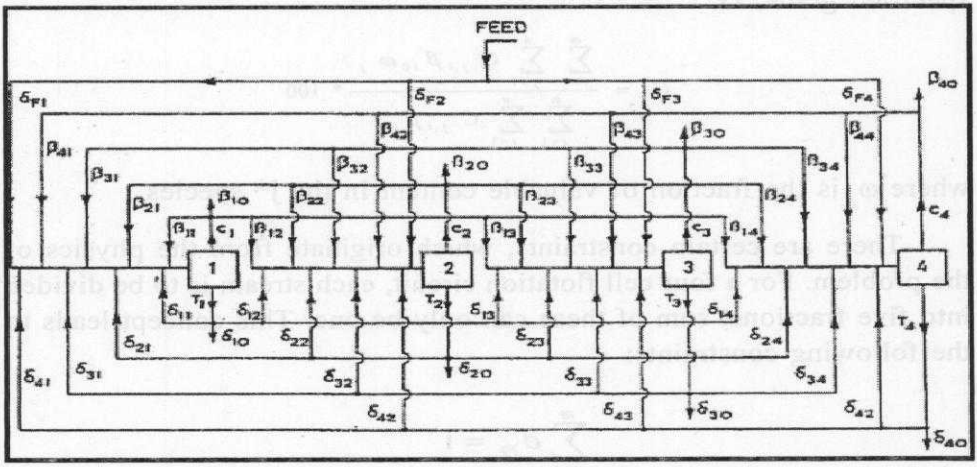


Fig 5. *Generalized configuration for four flotation cells.*

A typical raw material will have a valuable constituent and a gangue constituent - it may also have middlings. If this is the case, this raw material can be characterised in terms of three species. If we want to be more rigorous, we can characterise a given raw material in terms of larger number of species depending on how this raw material responds to a typical batch flotation test. Each species can be characterised in terms of its overall flotation constant as well as its chemical composition, particularly the percentage of the valuable constituent in it.

In the generalised configuration, the configuration coefficients β_{ij} and δ_{ij} refer to the fraction of concentrate and tailings, respectively, recycled from the jth cell to the ith cell. β^{o}_{j} and δ^{o}_{j} are the fractions of concentrate and tailings flow respectively, exiting from the jth cell as output. δ_{Fi} is the fraction of the new feed going to the ith cell.

Using an appropriate flotation kinetics model it is possible to calculate the mass flow rate of concentrate and tailing streams from each cell in terms of the configuration coefficients (betas and deltas), mean residence time in each cell, and the flotation rate constant for each species in the raw feed. Once the mass flow rate of each of the concentrate and tailing streams are known, one can define the percentage recovery (valuable component wise or overall recovery) as well as the grade of the concentrate. It is now possible to convert this problem into a constrained optimisation problem. For example, depending on the requirement, one may aim to maximise recovery subject to a minimum specified grade, G.

$$G = \frac{\sum_{i=1}^{m}\sum_{j=1}^{n} C_{j,i}\beta_{i0}\omega_j}{\sum_{i=1}^{m}\sum_{j=1}^{n} C_{j,i}\beta_{i0}} * 100$$

where ω_j is the fraction of valuable content in the j^{th} species.

There are certain constraints, which originate from the physics of the problem. For a four cell flotation circuit, each stream is to be divided into five fractions; sum of these can only be one. This concept leads to the following constraints:

$$\sum_{i=1}^{m} \partial_{i,i} = 1$$

$$\sum_{i=1}^{m} \partial_{ki} + \partial_{k0} = 1$$

$$\sum_{i=1}^{m} \beta_{ki} + \beta_{k0} = 1$$

$$0 \le (\delta, \beta) \le 1$$

$$0 \le \alpha_{ji} \le 1$$

Thus the generalised circuit problem is converted into a constrained optimisation problem to maximise recovery. We aim to find out alpha (α), betas (β) and deltas (δ) in such a way that the recovery is maximum, subject to a minimum grade of the product concentrate and the above physical constraints.

There are several algorithms, which may be used to solve this problem. We solved it by three different methods. First time in mid 70's,

we used random search method. Later on we solved it using the more sophisticated technique of Luse Jaccola and now we are trying to solve the same problem using an adapted version of genetic algorithm. Just for illustration purpose, I present one typical result for a feed consisting of 15% valuable, 20% middling and 65% gangue. Each of these species is characterised in terms of an apparent flotation rate constant and its chemical composition. Solution of this optimisation problem results in a circuit configuration shown in Fig. 6. No doubt, the circuit appears to be quite complicated wherein one of the streams is split into two parts; another stream is split into three parts and so on. It is beyond doubt that any additional stream in a plant would mean additional pipeline, pumping of slurry etc. and one has to pay a price for all this. However, this can be easily taken into consideration by imposing a penalty function for each additional stream. One can further simplify the circuit by imposing the condition that split streams with very small fractions can be neglected. The model since then has been validated using the plant data available in published literature and one of the operating plants in India.

Feed composition, %	Constraints	Values of the parameters
Valuable = 15	$G = 35$	$K_{val} = 1$/min
Middling = 20	$0 \leq \lambda_j \leq 20, j = 1, 2, \ldots, 4$	$K_{mid} = 0.1$/min
Gangue = 65	$d_p = 20$	$K_{gang} = 0.01$/min
	$V = 80$ cu ft	$M_T = 25$ lb/min

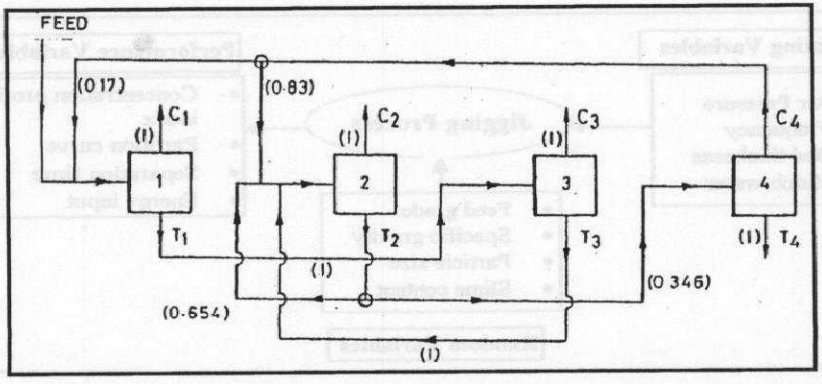


Fig 6. *Optimal configuration for three species, four cell problem*

Example 2 : Stratification of Particles during Jigging[3, 4]

Jigging is a process in which we try to beneficiate minerals by creating stratification of particulates in a pulsated slurry. We have a bed of solid particles and a mechanism for pulsating it - it could be a mechanical device or a hydraulic device or whatever else one can think of. When the bed is pulsated, during the pumping stage the slurry gets diluted and moves up and the entire bed opens up in a fluid medium. When the cycle is reversed, the particles settle down. When particles settle down in an aqueous medium, they have different settling behaviour depending on their density, morphology and size. This is the property that is used in a jigging process, where we try to separate out particles either based on their density, if the particles are of unisize or in terms of their size if the particles are of the same density.

Although the jigging process is over 400 years old, even today it is not properly understood. For the jig design also, people have used very different criteria and have come up with different design methodologies. While Japanese adopt a particular criterion for the frequency of pulsation and the amplitude, Russian and Americans adopt different criteria. We were curious to know how is that, jig performance does not vary much, even with different design criteria. To understand this, we realised that it would be necessary to understand the settling behaviour of particles and the process of stratification during pulsation of slurry.

In a typical jigging operation, one can identify four different stages, namely, inlet, expansion, exhaust and compression. In the inlet stage, the bed lifts up en masse. Near the end of the lift stroke, the particles at the

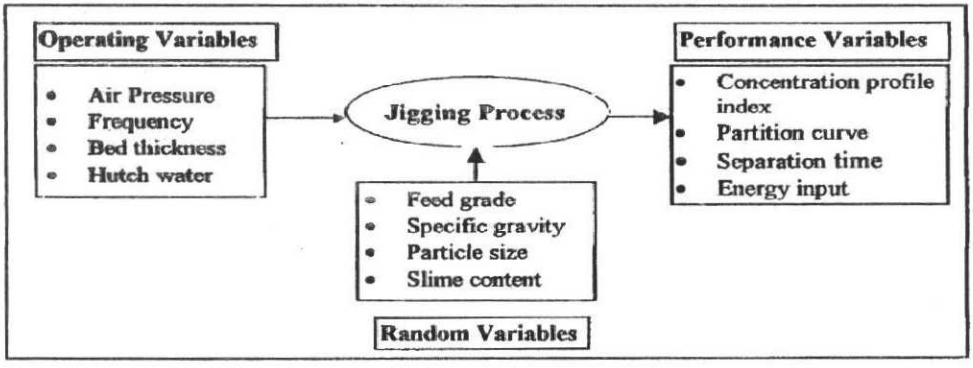


Fig 7. *Parameter affecting the stratification process in a jig.*

bottom of the bed start falling resulting in the loosening of the bed which in turn causes its expansion or dilation. During the third and fourth stages, the particles resettle through the fluid and the bed collapses back to its original volume. The pulsation and suction are repeated to bring about stratification with respect to specific gravity across the bed height. Various parameters affecting the stratification process are schematically shown in Fig. 7. These include amplitude and frequency of pulsation, bed thickness, and rate of hutch water flow and feed characteristics.

We have tried to study the jigging process using the Discrete Element Method (DEM). The jig model based on DEM essentially involves tracking the positions of each particle incrementally, applying Newton's Second law of motion and a force displacement law at the contact. A pair of springs and dashpots represents the contact. The success of this approach depends on an efficient scheme for identifying contacts and keeping track of them as time progresses. In order to achieve this, the whole experimental space is divided into a uniform cubical grid. The identity of each particle is mapped into these grids. In these cases where particles are considered as spherical elements, a particle can at most have entries in eight cubes, if the cube dimension is kept larger than that of the sphere. Thus, by checking each cube where the element has entry, all potential and existing contacts are identified. In calculating the contact forces, the elements are allowed to overlap.

We conducted a series of simulations by varying the amplitude and frequency of pulsation in a jig of 0.16 m diameter. Four hundred different balls of two different densities namely 2800kg/m^3 and 1500 kg/m^3 but of equal size (0.018 m diameter) and numbers were taken. All simulations

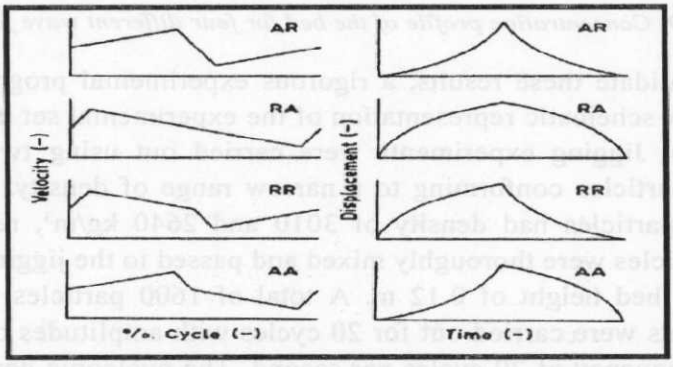


Fig 8. *Variation of fluid velocity and displacement with time for different types of wave forms.*

were done for 25 cycles. In order to analyse the effect of fluid wave forms on stratification, following wave forms (Fig. 8) were studied:

- AR (Accelerated upstroke and retarded down stroke)
- RA (Retarded upstroke and accelerated down stroke)
- AA (Accelerated upstroke and Accelerated down stroke)
- RR (Retarded upstroke and retarded down stroke)

The effect of these wave forms, as simulated by the DEM model, is presented in Fig. 9 in the form of concentration profile of the jig bed obtained after the end of the simulation.

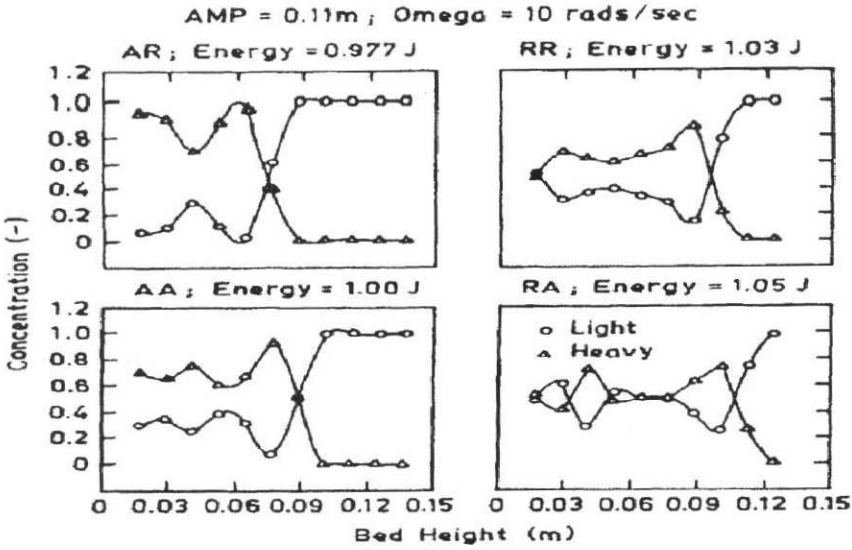


Fig 9. *Concentration profile of the bed for four different wave forms.*

To validate these results, a rigorous experimental programme was initiated. A schematic representation of the experimental set up is shown in Fig. 10. Jigging experiments were carried out using two types of artificial particles conforming to a narrow range of density. The heavy and light particles had density of 3010 and 2640 kg/m^3, respectively. These particles were thoroughly mixed and passed to the jigging chamber to make a bed height of 0.12 m. A total of 1600 particles were used. Experiments were carried out for 20 cycles with amplitudes of 5 and 10 cm and frequency of 20 cycles per second. The nucleonic density gauge was used to scan the bed height. The results of these experiments as well

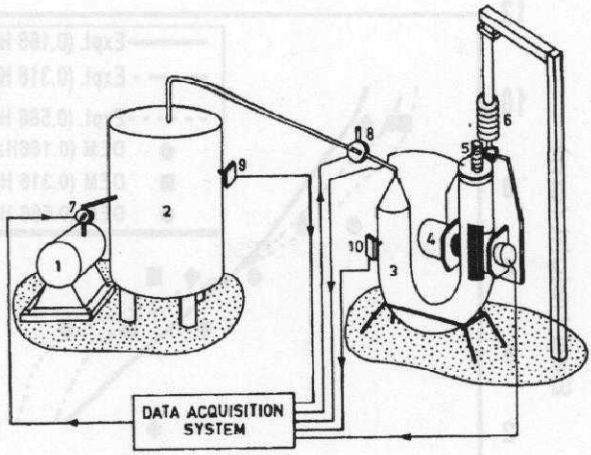


Fig 10. *Experimental setup showing locations of various equipments in the jig system. 1. Compressor, 2. Compensator, 3. Jig, 4. Nucleonic density gauge, 5. Level sensor, 6. Pneumatic actuator, 7. Two-way solenoid valve, 8. Three-way solenoid valve, 9. and 10. Pressure transducers*

as those of simulation are presented in Figs. 11 and 12. There is a reasonably good agreement between the model and the experimental data.

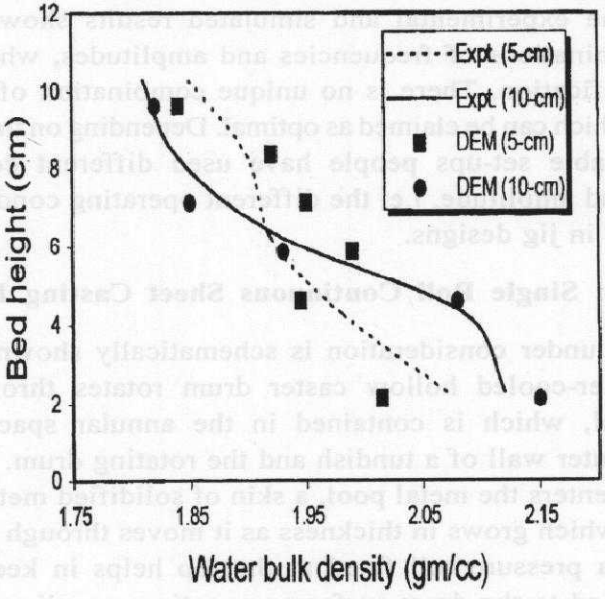


Fig 11. *Comparison between experimental data and DEM prediction for the density profile across the jig bed-effect of amplitude of pulsation.*

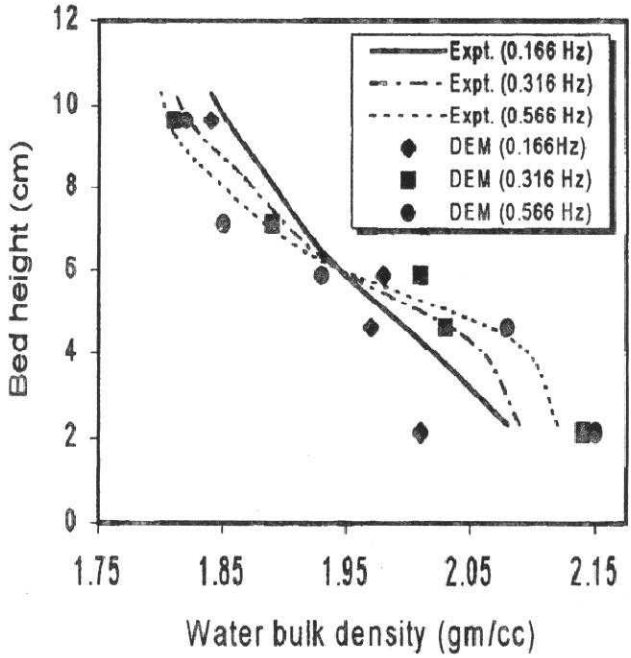


Fig 12. *Comparison between experimental data and DEM prediction for the density profile across the jig bed-effect of frequency of pulsation*

Both the experimental and simulated results show that there are several combinations of frequencies and amplitudes, which would give similar stratification. There is no unique combination of frequency and amplitude, which can be claimed as optimal. Depending on the characteristics of the available set-ups people have used different combinations of frequency and amplitude, i.e. the different operating conditions resulting in variations in jig designs.

Example 3 : Single Roll Continuous Sheet Casting Process[5-7]

The process under consideration is schematically shown in Fig. 13. In brief, a water-cooled hollow caster drum rotates through a pool of molten metal, which is contained in the annular space between the concentric outer wall of a tundish and the rotating drum. As soon as the caster drum enters the metal pool, a skin of solidified metal is formed on its surface, which grows in thickness as it moves through the metal pool. In Fig. 13, a pressure roll fixed at the top helps in keeping the sheet firmly attached to the drum surface preventing any slippage and also in maintaining uniform thickness of the sheet along the width. The sheet is separated from the drum surface by a knife edge.

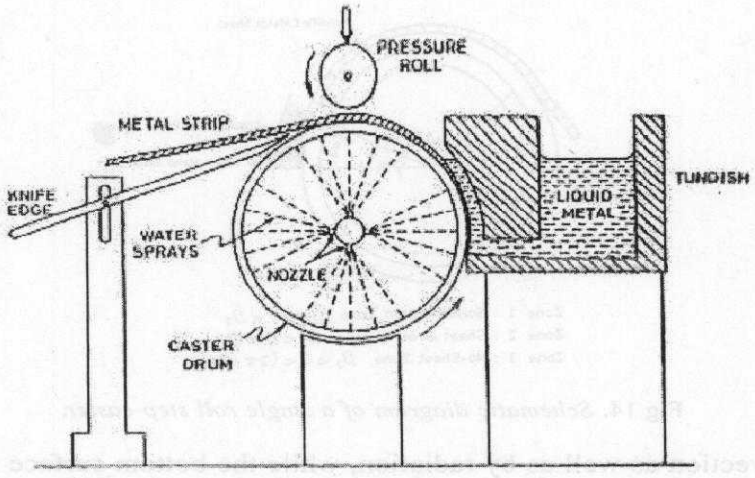


Fig 13. *Single roll continuous caster.*

Mathematical model

Development of a representative model describing the process has been an evolutionary exercise. Starting with a simple overall enthalpy balance model, we have come up with more rigorous mathematical model based on segment-wise heat balance, solidification and fluid flow considerations. Described below is the brief outline of the final model which is used for prediction and validation.

For modelling purpose, the system is divided into four distinct zones (Fig. 13): (i) liquid metal reservoir, (ii) liquid metal pool, (iii) solid sheet zone, and (iv) caster drum. As shown in the Fig. 14, in each rotation the caster drum passes through three different heat exchange zones.

1. Solidification zone ($\beta_1 < \theta < \beta_2$)
2. Sheet cooling zone ($\beta_2 < \theta < \beta_3$)
3. No sheet zone ($\beta_1 < \theta < (2\pi + \beta_1)$)

In the solidification zone, the caster drum moves through the metal pool. Its surface is covered by the solidified sheet, the thickness of which increases continuously as the drum moves from β_1 to β_2. In this zone, the heat flow is from the liquid metal pool to water sprays via solidified metal sheet and the caster drum. In the sheet cooling zone, the sheet has emerged from the liquid pool but is still attached to the drum. The top surface of the sheet transfers heat to the surrounding atmosphere

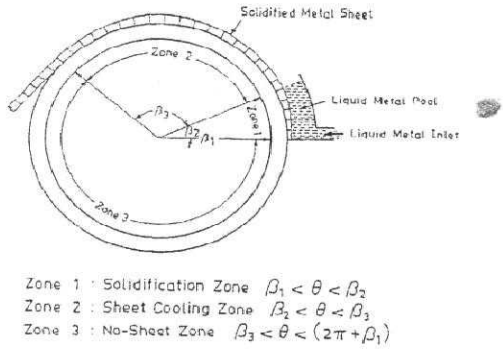


Fig 14. *Schematic diagram of a single roll step caster.*

by convection as well as by radiation, while the bottom surface attached to the caster drum transfers heat to the drum by conduction. As in the solidification zone, the heat from the caster drum is transferred to the water sprays. In the no sheet zone, the outer surface of the drum is exposed to the surrounding atmosphere and loses part of its heat to it. The model primarily consists of the momentum balance equations, which quantify the fluid flow phenomena in the molten metal pool and the energy balance equations for the metal pool, solidified strip and different zones of the caster drum. The 2-D momentum balance equation in steady state is written invoking the *equation of continuity* and the *vorticity transfer equation.* The concept of vorticity is used to combine the two components of momentum in r and θ directions into a single equation, and to eliminate the pressure term. The resulting equation contains two unknown velocity components v_r and v_θ. To reduce the number of unknowns, the concept of *stream function* is applied.

Separate energy equations are written for the molten metal pool, solidified metal sheet and different zones of the caster drum. For the molten metal pool, the steady state 2-D energy transfer equation is obtained from the generalised energy balance equation for laminar flow conditions for an isotropic fluid and assuming the conditions of negligible viscous dissipation. For the solidified metal sheet and different zones of the caster drum, the energy transfer equation is essentially the conductive heat transfer component of a generalised energy balance equation. All equations are written in the dimensionless form. Stream function and vorticity boundary conditions, and boundary conditions for energy transfer equations are specified. The model equations are solved numerically using an implicit finite difference technique to evaluate: (i)

stream function, (ii) velocity field in the molten metal pool, (iii) temperature field in the metal pool, solidified metal sheet and the caster drum and (iv) thickness of metal sheet. Model equations are solved for various sets of operating conditions. Some typical results are shown in Figs. 15-17.

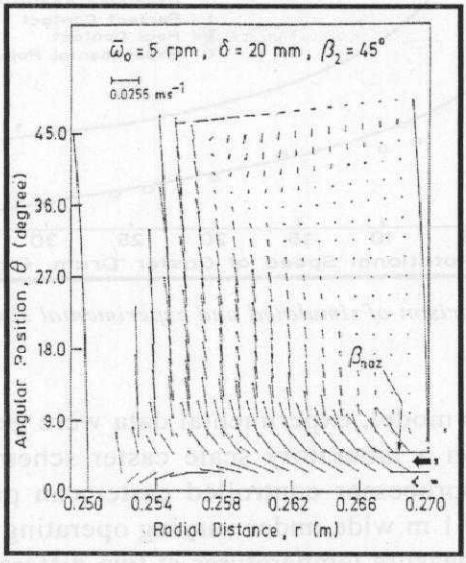


Fig 15. *Velocity field in molten metal pool.*

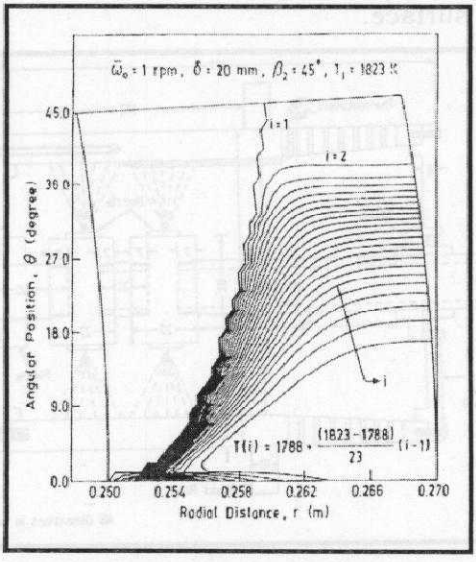


Fig 16. *Temperature isotherms in liquid melt.*

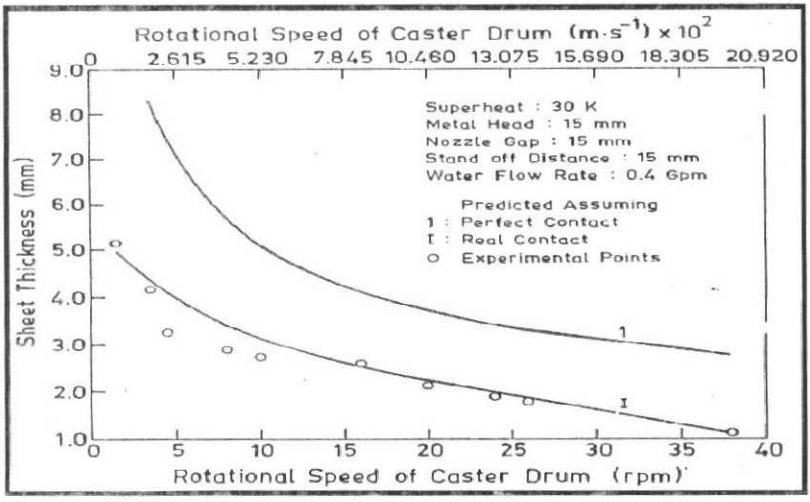


Fig 17. *Comparison of simulated and experimental sheet thickness.*

Experimental

To validate the model, experimental data were generated by casting aluminium sheets on a laboratory scale caster schematically shown in Fig. 18. This microprocessor controlled caster can produce continuous aluminium sheets, 0.1 m wide under varying operating conditions. It also has a provision to measure temperatures at two different locations in the caster - one very close to the outer surface of the caster and the other close to the inner surface.

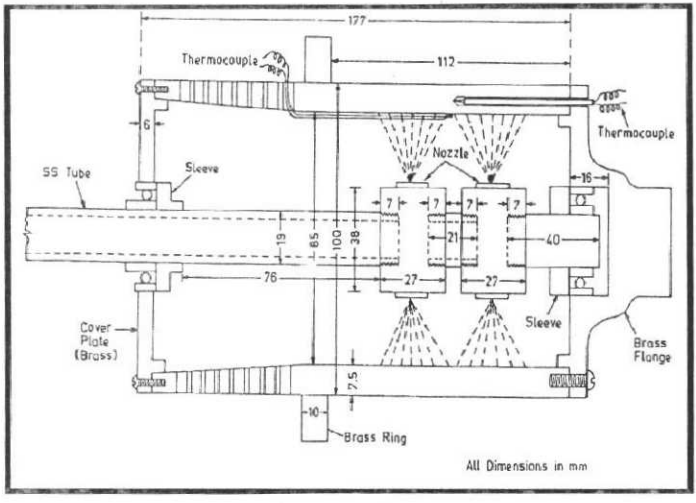


Fig 18. *Schematic diagram of caster drum assembly.*

Model Validation

Validation of the model using experimental data on sheet thickness for aluminium sheets produced under various conditions revealed large variations between the predicted sheet thickness values and those experimentally obtained. Re-examination of the model attributed this difference to the assumption of perfect thermal contact at the caster drum/ sheet interface. Perfect thermal contact essentially corresponds to infinite heat transfer coefficient. In reality, perfect thermal contact is not attainable for a variety of reasons. Imperfect thermal contact signifies a resistance to heat flow and the heat transfer coefficient, h_e, has a finite value implying different temperatures at the substrate and the casting side of the interface (Fig. 19). This more realistic mathematical description of heat transfer at this interface was incorporated by

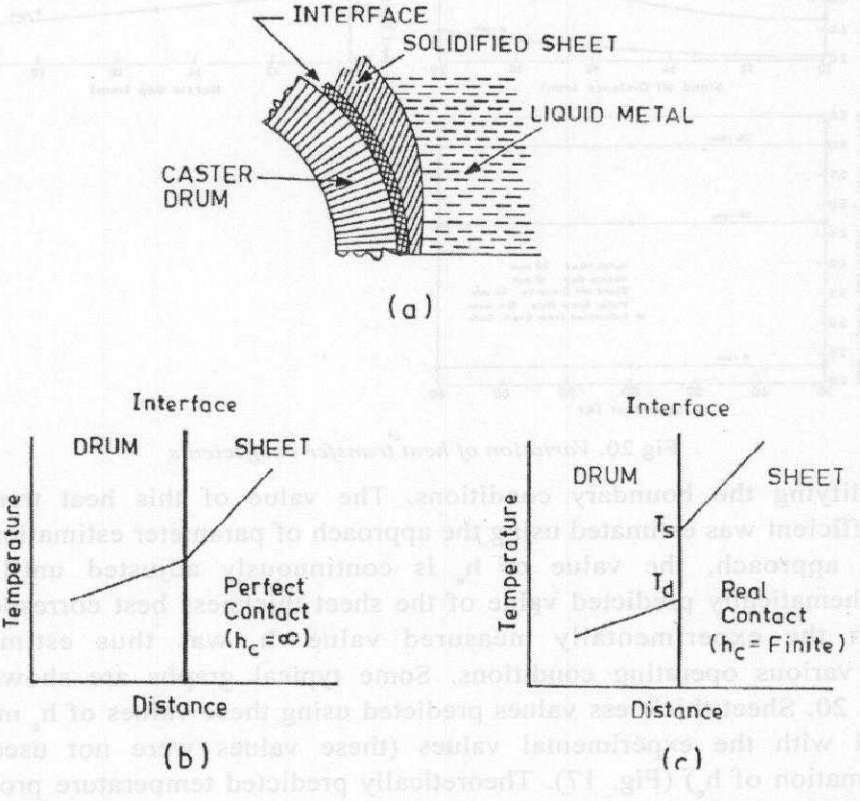


Fig 19. *Schematic temperature profiles in the metal sheet and the caster drum for perfect and imperfect/real thermal contacts.*

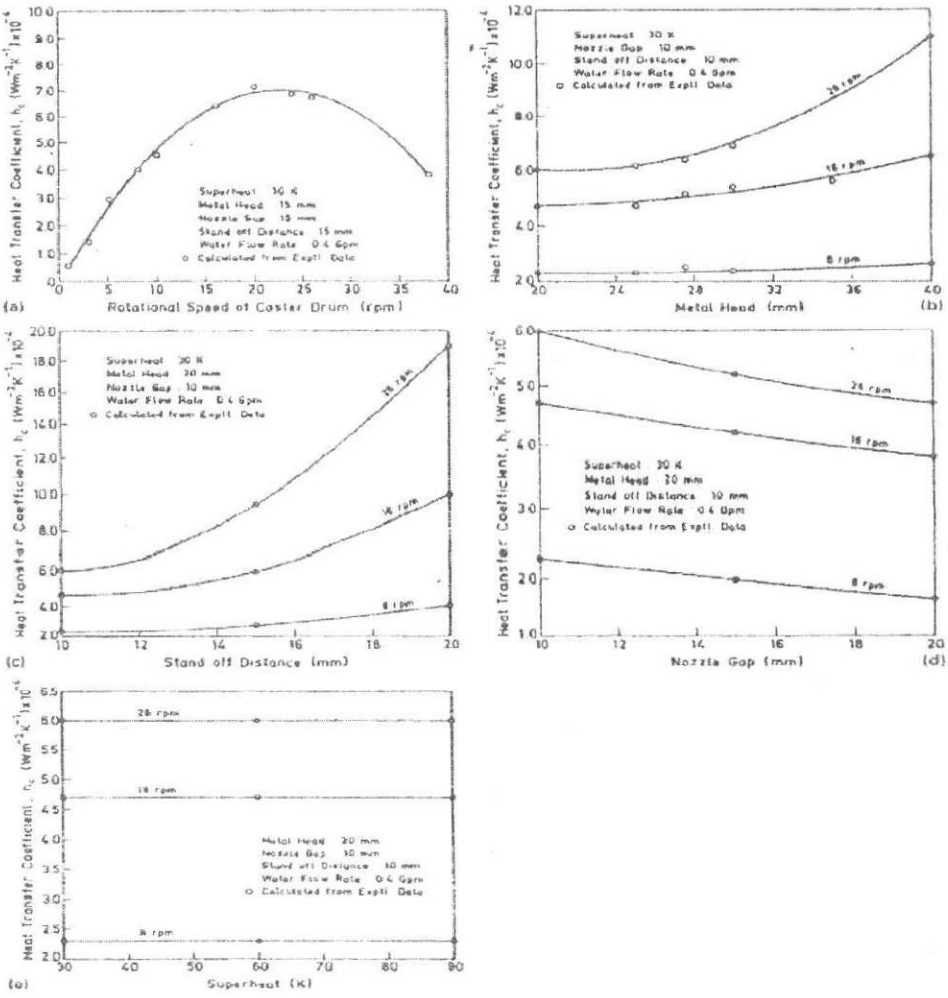


Fig 20. *Variation of heat transfer coefficients*

modifying the boundary conditions. The value of this heat transfer coefficient was estimated using the approach of parameter estimation. In this approach, the value of h_e is continuously adjusted until the mathematically predicted value of the sheet thickness best corresponds with the experimentally measured value. h_e was thus estimated for various operating conditions. Some typical graphs are shown in Fig. 20. Sheet thickness values predicted using these values of h_e match well with the experimental values (these values were not used in estimation of h_e) (Fig. 17). Theoretically predicted temperature profiles in the caster drum also match well with the temperature values recorded at two locations (Fig. 21).

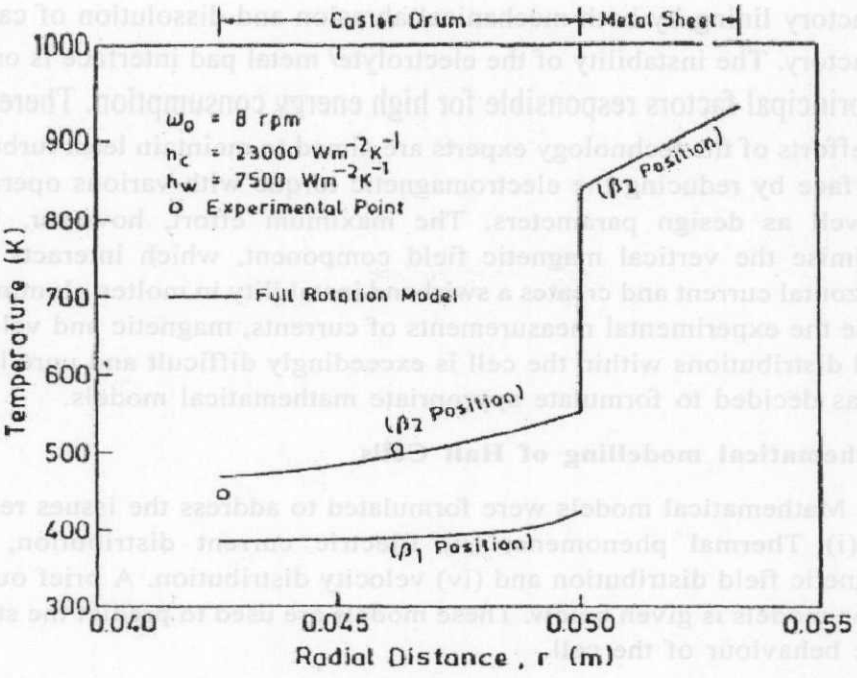


Fig 21. *Radial temperature profile for caster drum and aluminum sheets.*

Example 4 : Study of Magnetohydrodynamics in Hall-Heroult Cells[8]

In spite of the best efforts, even today the actual energy consumption in Hall cells is substantially higher than the minimum theoretical value needed for dissociation of alumina dissolved in cryolite to form aluminium metal and CO/CO_2 gas. There are several reasons for it, but the primary reason is related to magnetohydrodynamics phenomena in the cell. During the operation of the cell, two forces act on the electrolyte: (i) a force due to the interface momentum exchange arising from the anodic gas release (a buoyancy effect) and (ii) an electromagnetic force produced from the interaction between current and magnetic fields. Current flow in typical Hall cell varies between 150 - 250 kA, which produces a strong magnetic field within the cell. This magnetic field interacts with the flowing current to produce an electromagnetic force causing an electromagnetic torque, which provides motion to the conducting melts - the electrolyte and the aluminium metal pad. The electromagnetic force within the cell also causes a horizontal motion, which destabilizes the metal/ electrolyte interface leading to short circuiting of the aluminium pad and anode, and erosion of carbon

refractory lining by both mechanical abrasion and dissolution of carbon refractory. The instability of the electrolyte/ metal pad interface is one of the principal factors responsible for high energy consumption. Therefore, the efforts of the technology experts are aimed to maintain least turbulent interface by reducing the electromagnetic torque with various operating as well as design parameters. The maximum effort, however, is to minimise the vertical magnetic field component, which interacts with horizontal current and creates a swirl and instability in molten aluminium. Since the experimental measurements of currents, magnetic and velocity field distributions within the cell is exceedingly difficult and unreliable, it was decided to formulate appropriate mathematical models.

Mathematical modelling of Hall Cells

Mathematical models were formulated to address the issues related to: (i) Thermal phenomena, (ii) Electric current distribution, (iii) Magnetic field distribution and (iv) velocity distribution. A brief outline of the models is given below. These models are used to predict the steady state behaviour of the cell.

Thermal phenomena : Temperature distribution within the cell directly affects the geometric profile of the frozen cryolite crust (ledge profile) and the two together have a direct bearing on current efficiency, specific energy consumption, fluoride emission and even the anode consumption. A steady state two dimensional thermal model was formulated with primary objective to predict: (i) the ledge profile and (ii) temperature distribution within the entire cell including the carbon lining and the cathodic block. Thermal model treats conduction of heat within the sides and bottom of the cell as two-dimensional heat flow problem. Joule heat generation is taken as a heat source term in the heat conduction equation. All cell boundaries except for the ledge profiles are characterized once the cell configuration is specified. All boundary conditions are specified. The resulting model equation is solved for specified boundary conditions using a numerical method - we used the 'PHOENICS (Version 2.1.6)' software to solve the model equation. To start the solution, a ledge profile is assumed and the model equations are solved to give complete temperature profile, then the ledge profile is computed from the temperature isotherm which corresponds with electrolyte melting point. If this profile is different from the initially assumed, the model equations are re-solved for this new ledge profile. This iterative procedure is continued till the solution converges.

Electric current distribution : Electric current distribution in different regions of the cells is a critical factor in the development of thermal and hydrodynamic phenomena. Electric current along the bars generate the largest contributions to magnetic fields. The interactions of these fields with electric currents in the melt produces volumetric Laplace forces inducing movements in these melts. Joule heat generated by electric current flowing through the cell can be calculated by computing resistivity and current distribution within cell by application of Ohm's law.

The study of the electrical phenomenology can be divided into two central subjects:

1. Electrical current and potentials in volumetric conductors (anode, cathode and melts).

2. Current distribution in bars (anodic and cathodic bus bars, anodic and cathodic bars)

The 3-D potential (ϕ) and current distribution (J) within the cell can be calculated solving the following equations:

$$\frac{\partial}{\partial x}\left(\sigma\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\sigma\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\sigma\frac{\partial\phi}{\partial z}\right)=0$$

and $J=-\sigma\nabla\phi$

These equations were solved using 'PHOENICS' software for the specified boundary conditions.

Magnetic field distribution : Once the current density distribution within the cell is determined, magnetic field strength and direction at any point can be determined by application of Biot-Savart law in integral form. There are three sources of magnetic field (MF) in the cell.

1. Electric currents in the bars (bus bar, anodic and cathodic bars, etc)
2. Electric currents in volumetric conductors (anodes, melts and cathodic blocks).
3. Steel parts (cell shell).

MF originated from electric currents in the bars can be computed applying Ampere's law to rectilinear conductors of negligible cross

section area and finite length. MF from anodes, melts and cathodes is computed by integration of the volumetric current density flowing through these. MF from volumetric conductors can also be computed solving the Laplace equation for scalar potentials.

Velocity field distribution model : Mathematical description of the movements of the melts in the cell (cryolitic bath and molten aluminium) is a complicated task. Two layers of viscous fluids are superposed; their movement is turbulent in certain regions of the cell. The cryolitic bath is agitated by the electromagnetic forces and the movements of CO_2 and CO. We neglected the latter effect in our model which is based on the Navier-Stokes equation of motion and the equation of continuity. The electromagnetic force is taken as the source term. The shallow water approximation is invoked for the melt which introduces depth averaged velocities.

Model Predictions

Model formulations described above may be used to calculate thermal profile, current distribution, magnetic fields and velocity distributions for industrial Hall cells. We made computations for one such cell but could not validate our results as there was no provision in the cell to measure these quantities. We therefore decided to set up a laboratory scale simulated Hall cell in which woods metal was used as the liquid phase. The basic idea was to use this set-up to generate large amount of experimental data which could be used to validate the model predictions. Therefore, subsequently, all the model predictions were made for different experimental conditions used in this simulated cell. A few typical results are presented in the following section.

Experimental Set-up

The low temperature simulated multi-anode Hall cell is schematically shown in Fig. 22. The cell consists of:

(i) Inner stainless steel box, which represents the cavity of Hall cell and can hold upto 50 kg of simulating liquid, that is woods metal, which was selected because of its low melting point of ~75°C and high electrical conductivity.

(ii) Anode assembly: Six stainless steel blocks suspended from anode bus bar by copper rods simulate the carbon anodes.

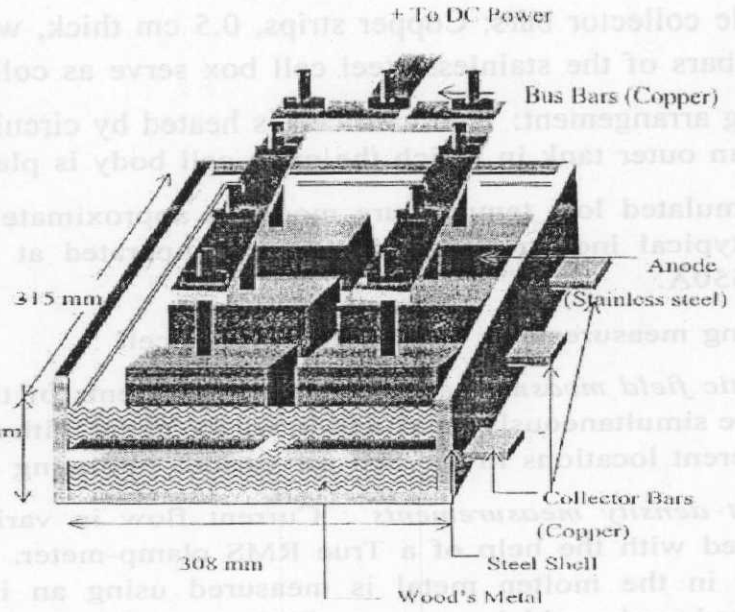


Fig. 22. *(a) Schematic diagram of low temperature simulated Hall cell*

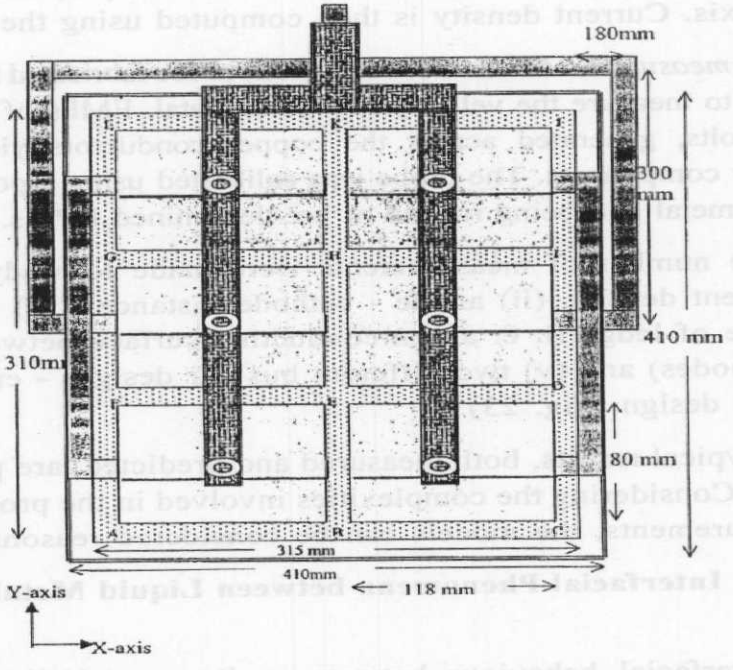


Fig. 22(b). *Top view of bus bars attached to anodes for end riser design.*

(iii) Cathode collector bars: Copper strips, 0.5 cm thick, welded to the inside bars of the stainless steel cell box serve as collector bars.

The simulated low temperature model is approximately one-tenth scale of a typical industrial cell and can be operated at a maximum current of 550A.

The following measurements were made in this cell :

1. *Magnetic field measurements :* Three components of the magnetic field are simultaneously measured in woods metal with a Hall probe at different locations in the cell for various operating conditions.

2. *Current density measurements :* Current flow in various bars is measured with the help of a True RMS clamp-meter. The current density in the molten metal is measured using an indigenously fabricated probe which measures EMF drops between two sets of conductors, each set having two conductors. Line joining one set of conductors represents X-axis, while the other, perpendicular to it, is Y- axis. Current density is then computed using the Ohm's law.

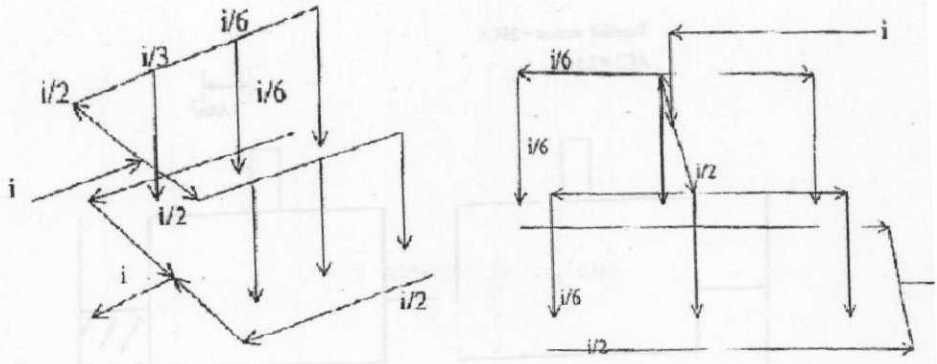
3. *Velocity measurements :* An electromagnetic probe fabricated indigenously, is used to measure the velocity in woods metal. EMFs of the order of nano volts, generated across the copper conductors yield the two velocity components. The probe was calibrated using a pot containing Woods metal and being rotated at pre-determined RPMs.

A large number of measurements were made to study the effect of - (i) current density, (ii) anode - cathode distance, (iii) cold anode, (iv) presence of ledge (i. e. a non-conducting surface between the cell walls and anodes) and (v) two different bus bar designs - end riser and quarter riser design (Fig. 23).

Some typical results, both measured and predicted, are presented in Figs. 24-26. Considering the complexities involved in the process as well as the measurements, the models can be considered reasonable.

Example 5 : Interfacial Phenomena between Liquid Metal - Ceramic Substrates[9]

The interfacial behaviour between molten metal/alloy and solid ceramic substrate is of great industrial significance because of its bearing



(a) Schematic drawing of the end riser design. (b) Schematic drawing of the quarter riser design.

Fig 23. *End riser and quarter riser bus bar designs.*

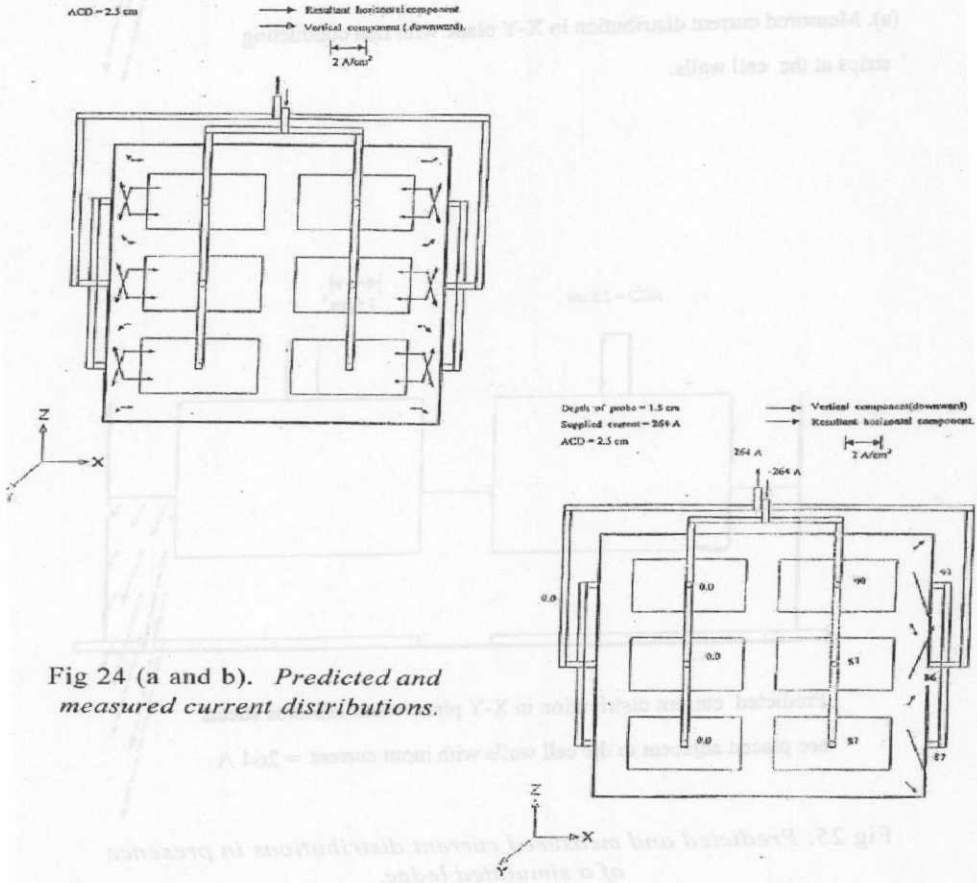
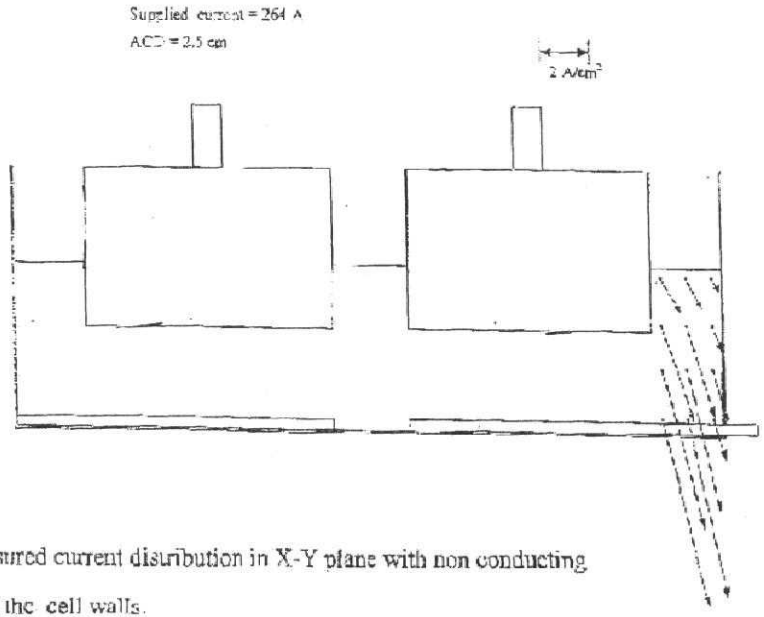
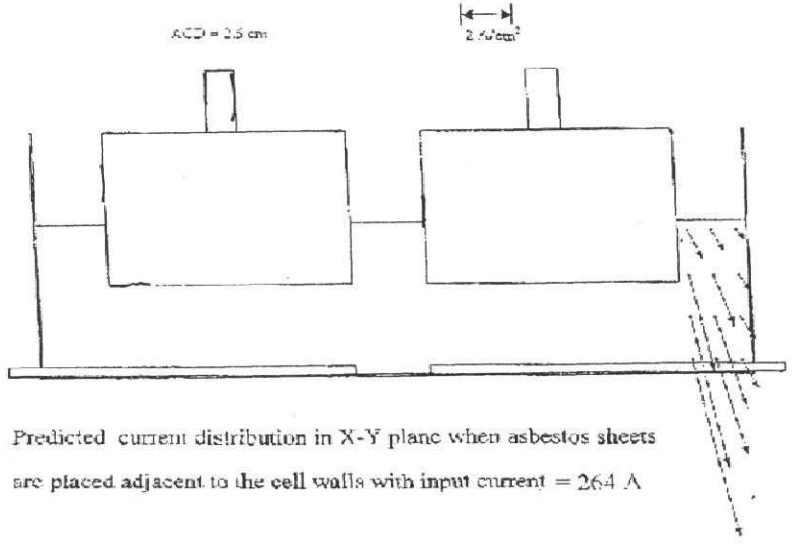


Fig 24 (a and b). *Predicted and measured current distributions.*

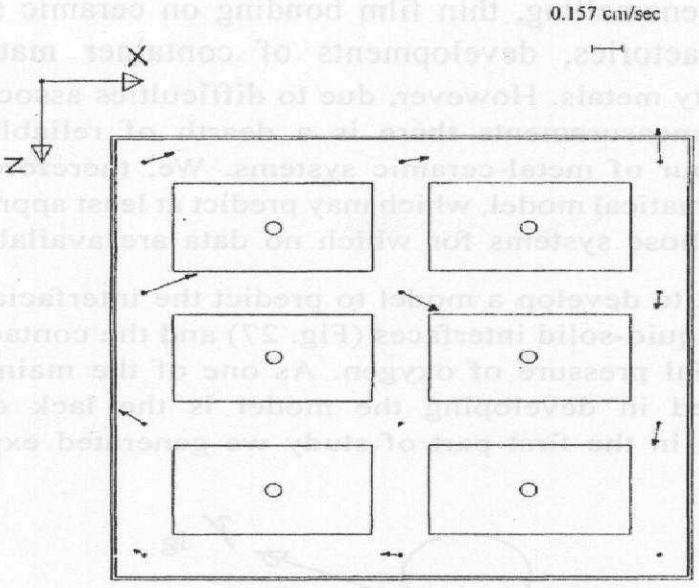


(a). Measured current distribution in X-Y plane with non conducting strips at the cell walls.

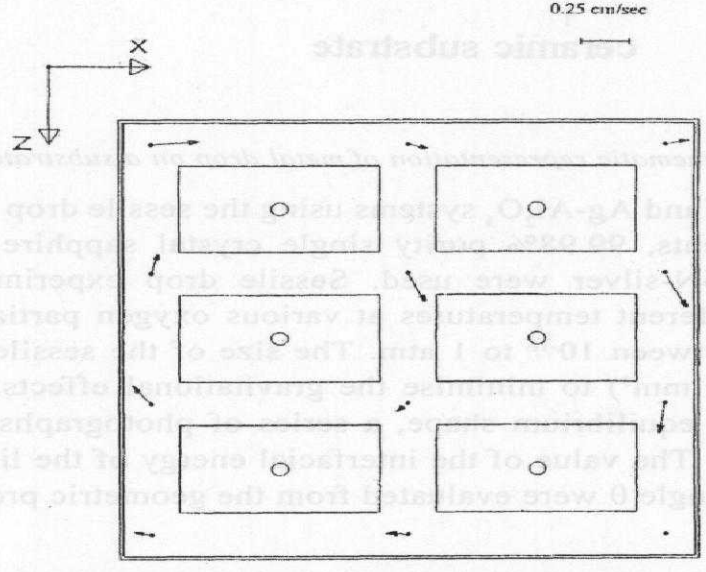


Predicted current distribution in X-Y plane when asbestos sheets are placed adjacent to the cell walls with input current = 264 A

Fig 25. *Predicted and measured current distributions in presence of a simulated ledge.*



(a) Measured velocity distribution in end riser design in X-Z plane with current input 288 A at Y = 0.6 cm.



(b) Predicted velocity distribution in end riser design in X-Z plane with current input 288 A at Y=0.6 cm

Fig 26 (a & b) *Predicted and measured velocities.*

on processes like enamelling, thin film bonding on ceramic substrates, corrosion of refractories, developments of container materials for smelting high purity metals. However, due to difficulties associated with the experimental measurements there is a dearth of reliable data on interfacial behaviour of metal-ceramic systems. We, therefore, decided to develop a mathematical model, which may predict at least approximately, the behaviour of those systems for which no data are available.

We attempted to develop a model to predict the interfacial energies at liquid-gas and liquid-solid interfaces (Fig. 27) and the contact angle as a function of partial pressure of oxygen. As one of the main problems that is encountered in developing the model is the lack of reliable experimental data, in the first part of study we generated experimental

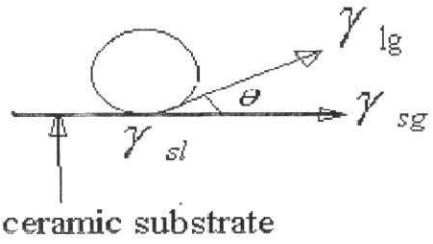
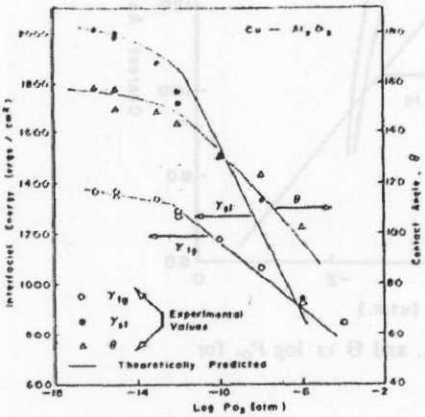


Fig. 27 *Schematic representation of metal drop on a substrate.*

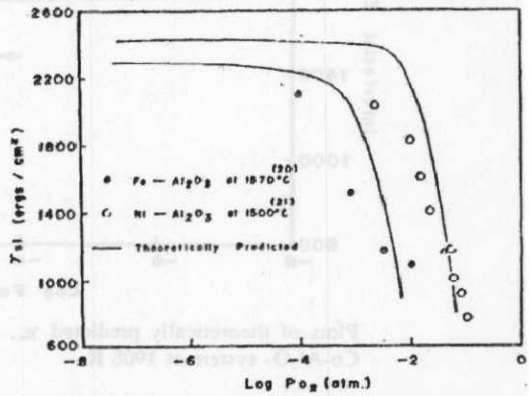
data for Cu-Al_2O_3 and Ag-Al_2O_3 systems using the sessile drop technique. For the experiments, 99.98% purity single crystal sapphire substrate, 5N-copper and 5N-silver were used. Sessile drop experiments were carried out at different temperatures at various oxygen partial pressure values ranging between 10^{-16} to 1 atm. The size of the sessile drop was kept small (~ 6.3 mm^3) to minimise the gravitational effects. Once the drop attained the equilibrium shape, a series of photographs of sessile drops were taken. The value of the interfacial energy of the liquid metal (γ_{lg}) and contact angle θ were evaluated from the geometric profile of the sessile drop.

In developing the model it is assumed that the interfacial energy of the ceramic substrate (γ_{sg}) is a function of temperature only, and that the interfacial energy of pure liquid metal (γ_{lg}) is either known or can be estimated. The approach that is used here in developing the model involves two main steps. The first step is to develop a relationship between

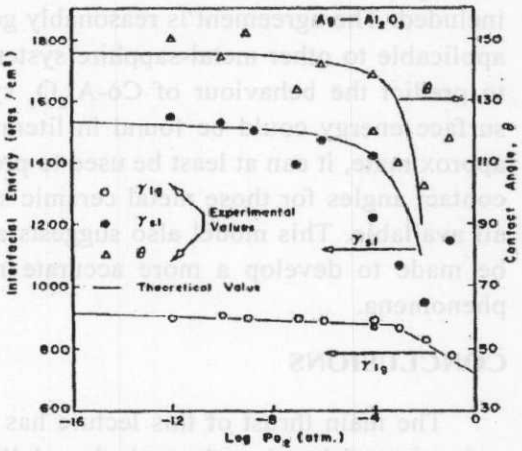
γ_{lg} and Po_2. An attempt is then made to express the contact angle θ as a function of either γ_{lg} or γ_{sl} so that when the expression for γ_{lg} and θ are substituted in Young - Dupre equation [$\gamma_{sl} = \gamma_{sg} - \gamma_{lg}\cos(\theta)$] the resulting equation is a relationship between γ_{sl} and Po_2 (or γ_{sl} and θ). This enables one to predict γ_{lg} and γ_{sl} as well as θ as a function of Po_2 just from the knowledge of a few fundamental parameters, e.g. the free energy of formation of the compound at the liquid metal-ceramic interface, or the work of adhesion. The free energy of formation data is available for several metal-ceramic systems. Similarly, work of adhesion data are either available or can be estimated for many systems.



Plots of theoretically predicted γ_{lg}, γ_{sl}, and Θ vs log P_{O_2} for Cu-Al_2O_3 systems at 1423 K. Experimental values are also shown.



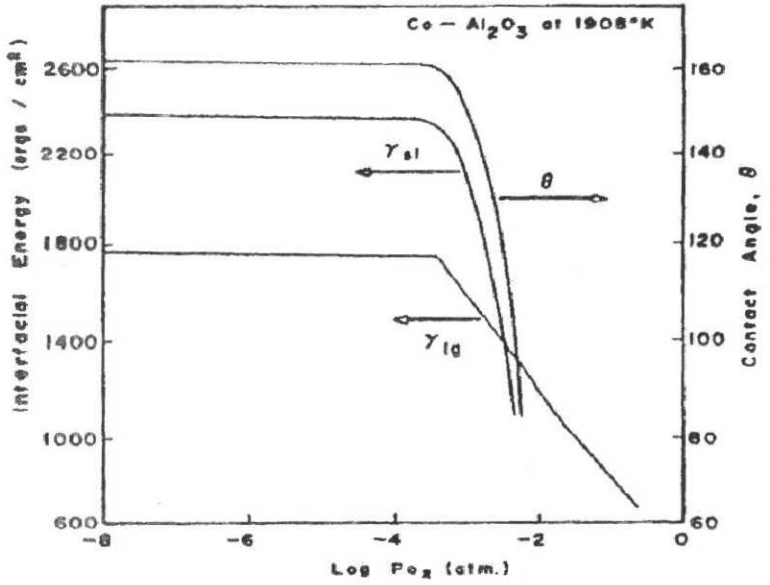
Plots of theoretically predicted γ_{sl} vs log P_{O_2} for Fe-Al_2O_3 system at 1843 K and for Ni-Al_2O_3 system at 1773 K. Experimental values are also shown.



Plots of theoretically predicted values of γ_{lg}, γ_{sl}, and Θ vs log P_{O_2} for Ag-Al_2O_3 system at 1258 K. Experimental values are also shown.

Fig 28 *Plots of, and as a function of for Cu-Al_2O_3, Ag-Al_2O_3, Fe-Al_2O_3 and Ni-Al_2O_3 systems.*

To test the validity of the model, variation in γ_{lg}, θ and γ_{sl} as function of $\log(Po_2)$ are predicted for Cu, Ag, Fe and Ni. Theoretically predicted plots of γ_{lg}, θ and γ_{sl} vs $\log (Po_2)$ are shown in Fig. 28 for Cu-Al_2O_3 and



Plots of theoretically predicted γ_{lg}, γ_{sl}, and Θ *vs* log P_{O_2} for Co-Al_2O_3 system at 1908 K.

Fig 29 *Predicted interfacial energies for Co-Al_2O_3 System.*

Ag-Al_2O_3 systems, where the experimentally determined values are also included. The agreement is reasonably good. Assuming that the model is applicable to other metal-sapphire system as well, an attempt was made to predict the behaviour of Co-Al_2O_3 system in Fig. 29, for which no surface energy could be found in literature. Even if the model is only approximate, it can at least be used to predict the interfacial energies and contact angles for those metal ceramic systems for which no data are at all available. This model also suggests a direction in which efforts may be made to develop a more accurate model for predicting interfacial phenomena.

CONCLUSIONS

The main thrust of this lecture has been to illustrate how effective and a powerful tool mathematical modelling can be in developing a better understanding of the physical/chemical phenomena and simulating a

process if this tool is used intelligently and judiciously. With the help of five examples I have attempted to establish that for a good and meaningful modelling activity, an intelligently designed experimental programme is of paramount importance. No matter how precisely the model equations are formulated, and assumptions are validated, no matter how sophisticated software packages are used to solve the model equations, the accuracy of the final results depends on the accuracy and reliability of the values of the parameters used and the precision with which the boundary conditions are characterized. For many real life systems and processes, the latter two are obtained through experimental measurements. It is therefore strongly advocated that a judicious experimental programme must always be an integral part of any meaningful mathematical modelling programme.

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