Building Useful and User-Friendly Computer Models of Metallurgical Processes

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INTRODUCTION

Industrial processes in the metallurgical field are complex by nature; they are also costly to build and operate. It is, therefore, worthwhile or even necessary to develop mathematical models for the purpose of process analysis or design. However, to be representative, the model must also be complex, and model building itself becomes a sizeable undertaking. As a result, model building and model use have gradually become two separate engineering activities—rarely are model builders and model users the same people. Usually, model builders are academic and laboratory workers; model users, on the other hand, tend to be industrial researchers or process engineers.

In tandem, two ongoing developments are fueling an upsurge in mathematical modeling activities, especially as related to complex, large-scale models that require sophisticated numerical and algorithmic developments and sizeable data-processing capacities. First is the ever-increasing availability of powerful computers that are faster and cheaper than their predecessors. Second is the maturation of a variety of general-purpose codes for different applications.

With new hardware and software tools opening horizons to academic and industrial workers alike, now more than ever there is a need for cooperative endeavors—the model builder must fully understand the needs and expectations of the model user, and the model user must be aware of the constraints and limits that bind the model builder. In many ways, a lack of understanding about these issues is the source of conflict. For example, code users often say code builders underestimate the users' needs; code builders suggest users underestimate learning curves and/or expect too much from current technology. Model builders frequently experience conflict since they are also code users (general-purpose codes are used to build models).

For the sake of successful technology transfer and progress in the field, a collaborative approach must be taken by model builders and users.

THE PHYSICS OF INDUSTRIAL PROCESSES

Most industrial metallurgical processes are transformation processes, whereby the goal is to transform a raw material into a final product with added value. The processes are largely thermohydrodynamic in nature, involving heat transfer and fluid flow at high temperatures. They may also involve mass transfer, phase-changes, interphase heat transfer, interphase transport, radiative-energy transfer in an absorbing, emitting, transmitting, or scattering medium, free surface flow, porous media flow, solu­

tional convection, chemical reaction, combustion, electromagnetism, magnetohydrodynamics, or fluid-solid interaction.

Each of these areas, taken separately, is a contemporary research domain of some note. Fortunately, no industrial process is complicated enough to incorporate all of these phenomena; however, processes involving several are legion in the metallurgical industries. The phenomena often occur in a simultaneous and interactive manner, with one effect controlling the other and vice-versa. The case most frequently encountered is interactive fluid flow and heat transfer, but there are many other common examples as well.

In the process of baking the carbon electrodes used in the electrolysis of alumina for aluminum production, horizontal or vertical flue ring furnaces are used. Here, during carbon baking, such volatile substances as methane, hydrogen, and tars are produced. This evolution is a function of baking temperature and heating rate. The evolved volatile matter burns in the flue and this combustion, in turn, affects baking. Another example is found in the calcining of petroleum coke in rotary kilns. Once again, volatile matter is evolved; the effect is further complicated, however, as coke dusts are generated from the granular bed and burn in the freeboard gas if favorable conditions are met. This is another interactive phenomenon where gas
flow affects dust generation, entrainment, and combustion; these, in turn, affect gas flow. Another well-known example involves the melting of metal and is fundamentally referred to as the phase-change problem. The heating and melting of the solid charge modifies the solid-liquid boundary and, consequently, the flow field of the liquid metal. This, in turn, affects the convective heat transfer from the liquid metal to the solid charge and, therefore, the melting rate.

Industrial processes are usually large in dimensions, requiring costly and sizeable pieces of equipment. For example, it is not uncommon for a baking furnace to occupy the entirety of a building 200 meters long. Many of the processes are also slow, with time constants ranging from days to weeks.

For the modeler, the metallurgical processes’ hostile environments (including moving parts), complexity, and scale make it difficult to perform direct experimental studies or conduct plant monitoring, even with instruments. Further, cost is a powerful deterrent to trial-and-error investigations.

Despite these drawbacks, it is critical to realize that even a minor change in design or operational parameters could significantly improve the efficiency of a process. For example, many processes are energy consumers and even a small improvement in energy efficiency could translate into appreciable savings.

With in-plant experimental studies being difficult or, in some cases, impossible to conduct, a viable alternative is to build mathematical models and carry out simulations on computers.

**GENERAL-PURPOSE CODES**

Among the user needs reviewed in the “Expectations and Limitations” sidebar, the most prominent ones are ease of use and reasonable computing time. Hindering ease of use are a number of constraints, especially the complexity of the mathematics and model structure. Here, the advent of general-purpose codes has been a great help.

More than a decade ago, it became clear that it would be unrealistic to build a code to solve each class of modeling problems—the resulting profusion of codes would be difficult and expensive, to maintain and update. Thus, the trend was toward developing efficient, general-purpose codes based on the general form of a pertinent equation, such as the conservation equation. In this example, the specifics of a given problem are accounted for by the conservation law equations that are solved for the exchange coefficient, inclusion of appropriate source terms, and, possibly, a coupling with other subroutines created to simulate the problem. The general conservation equation is often written as

\[
\frac{\partial}{\partial t}(\rho \phi_i) + \nabla \cdot (\rho \mathbf{V}_i \phi_i) = r_i S_i
\]

where \(r_i\) is the volume fraction of phase \(i\), \(\rho\) is the density of phase \(i\), \(\phi_i\) is the conserved property of phase \(i\), \(\mathbf{V}_i\) is the velocity vector of phase \(i\), \(\Gamma_i\) is the exchange coefficient for \(\phi_i\), and \(S_i\) is the source of \(\phi_i\) per unit phase volume. The equation can be solved for mass, momentum (velocities), enthalpy (temperatures), species (concentrations), or other properties.

For mass conservation, using the code PHOENICS, \(\phi_i\) is equal to 1, the exchange term disappears, and the source term is given by the mass flow entering the phase per unit volume. For momentum conservation, \(\phi_i\) represents each of the space components of velocity; therefore, there are three equations for each phase. \(\Gamma_i\) is viscosity, and the source term \(S_i\) can contain such factors as pressure gradient, gravity force, friction force, electromagnetic force, centrifugal force, and terms resulting from coordinate rotation. For energy conservation, \(\phi_i\) is taken as the specific enthalpy of the phase, \(\Gamma_i\) is the thermal conductivity divided by the constant-pressure specific heat, and the source term \(S_i\) contains the variousheat sources or sinks, radiative heat fluxes, ambient heat losses, interphase heat transfers, or time-variations of source term.

**MODEL BUILDING**

With the application of general-purpose codes being the first step in building models that meet users’ needs, the