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Chapter 8. Process Modeling

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ABSTRACT

Mathematical process models can assist process development and optimization in many different ways. This chapter discusses the different types and attributes of process models, and offers some ideas to consider when developing, using, and implementing them. Process models range from empirical to mechanistic in nature and vary in complexity from simple analytical solutions to coupled, 3-D transient numerical simulations. They are classified here according to the way in which they are implemented in practice, viz. fully-online models, semi-online models, off-line models, and literature models. The purpose of the model should dictate how choices are made during its development. Ways to validate and compare the model with experiments are suggested. Examples are taken in the context of the authors' experience in modeling the continuous casting of steel.

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1. INTRODUCTION

The silicon chip has changed our approach to process analysis. In an earlier time, some of us actually used a slide rule and drew graphs by hand. There were merits in some of this as we learned to estimate, carry powers of ten, and think about what we were plotting. But, of course, the complexity of real processes eluded us, as only simple balances and analytical solutions were possible.

The burgeoning evolution of the computer and user-friendly software has fundamentally transformed our approach to process analysis and propelled us into the development and application of mathematical process models. The computer has unshackled us from the need to oversimplify. But improperly applied, it threatens to confuse and overwhelm us with needless complexity.

In this chapter on process modeling, the challenge to simplify complex processes while maintaining a strong hold on reality is addressed. As shown in Figure 8.1, we need to balance the mind-set of simplification with the power of complex analysis. And underpinning modeling must be measurements.

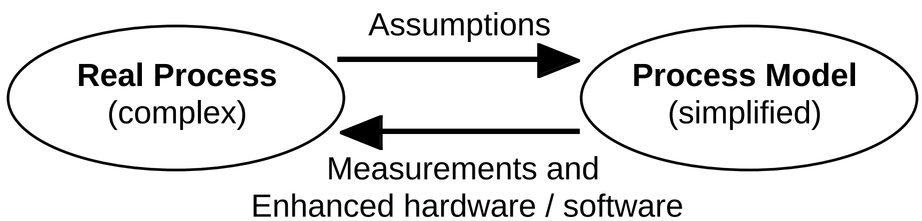

Figure 8.1. Compromise between mathematical simplifications, which push the process model away from reality, and tools which bring it closer

1.1. What is a process model?

A process model is a system of mathematical equations and constants that are usually solved on a computer to make quantitative predictions about some aspect(s) of a real process. The specific variables required as input data and generated as output predictions are important features of the model. The equations often stem from a numerical solution to one or more differential equations and their boundary conditions.

The model also includes the constants, which represent material properties, empirical relationships, and other knowledge about the process. These usually require considerable effort to obtain, normally by experimentation. Thus, general-purpose commercial software packages, (e.g. finite-element or finite-volume based codes), are not models in this context. They serve as useful tools, however, by providing frameworks for the development of process models, possibly saving effort in formulating the equations.

Thus, by definition, models require a combination of mathematics and experimental data. To be relevant, they also need to be validated with realistic measurements and finally implemented into practice. These aspects of process models will be treated in subsequent sections, in the context of examples taken from the continuous casting of steel, which is described in Chapter 12.

2. WHY MODEL?

There are many different reasons to develop a process model. These include:

- increase fundamental understanding of a process

- assist in scale-up
- design of experiments
- evaluation of experimental results
- quantifying property measurement
- online process control and optimization
- technology transfer

If a clear reason to develop a model cannot be found, then it should not be developed!

2.1 Increase process understanding

Perhaps the most important reason for modeling is to gain fundamental understanding of a process. Without this understanding, improvements can be made only by expensive trial and error, and error is more likely. Models can serve as off-line tools to correct misconceptions, identify what is important, test hypotheses and perform parametric studies. A validated process model is an ideal tool for isolating the effects of individual phenomena, because each variable of interest can be changed systematically and independently. Off-line study of the influence of different variables on the operation of a process is often the first step in process optimization.

2.2 Scale-up and design

Models are particularly important in the design of new processes and plants. The ability to extrapolate knowledge generated from bench-scale or pilot plant experiments to a commercial scale operation varies in direct proportion to the accuracy of the process model(s) used. Because there is no existing plant for calibration, it is crucial that models used for this purpose be as mechanistic as possible.

2.3 Design of experiments

Process models can help with experimental design in several ways. One way is to identify the critical location(s) in a process where measurements should be made, in order to get the most use from the experiment. For example, without the aid of a model, thermocouples might be placed needlessly in locations that are not very interesting. Alternatively, there may be too few thermocouples at critical locations where temperatures change rapidly.

Another use of a model is to help identify the process variables which are most critical, or rate-limiting. Experiments can then focus on quantifying the effects of just these variables. Finally, models can help to ensure that an experiment does not forget a crucial phenomenon, which governs the real process.

2.4 Evaluation of experimental results

Off-line process models can help to interpret the results of experiments. For example, temperature measurements may be converted to heat fluxes with the aid of a model. These heat fluxes enable more meaningful comparison between experimental results, because they are less specific to a particular experimental setup.

Process models are particularly useful when the phenomena are difficult to measure or model physically. Examples relevant to continuous casting include flow in the liquid pool generated by electromagnetic or thermal effects, and thermal stress generation. A good process model can extrapolate the results from a few key experiments to other conditions and help to find the optimal process conditions with less experimental effort.

2.5 Property measurement

Models are very important in the measurement of properties. This is because properties are not measured directly, but are instead derived from measurements using a model. Furthermore, particular property data must only be used with the specific model used to extract it from the raw measurements.

For example, thermal conductivity is typically calculated from an experiment which measures two temperatures and the distance between them for a known applied heat flux. Generally, a simple form of Fourier’s heat conduction law is used to extract the thermal conductivity. If, however, the material is a semi-transparent slag, for example, then the measurements will include heat transmitted by both conduction and radiation. The conductivity calculation may or may not account for this radiation. Thus, several different conductivity “measurements” are possible from the single experiment, depending on the heat transfer model employed in the property calculation. A sophisticated model might even combine the results from several experiments to simultaneously calculate the thermal conductivity and the radiation absorption coefficient.

Future process models using the “measured” conductivity should separately account for radiation or not, according to the same heat transfer model employed in the property calculation. Obviously, it is important that the experimenter reporting the property “measurements” clearly indicate the model used in calculating the property data.

This particular example arises when quantifying the thermal properties of molten slag layers. Similar difficulties arise during measurement of other properties, whenever there are complicating phenomena which cannot be avoided in the experiment. Other practical examples include inelastic creep relaxation during the measurement of elastic modulus at high temperature; and strain localization during the measurement of critical fracture strain. The lack of complete, fundamental property data, in areas such as these, is one of the many factors limiting the accuracy of current process models.

Models can contribute to property measurement by providing a framework common to experimenters and modelers alike. The need for general models of fundamental material behavior is growing, as the phenomena of interest grow in complexity and experiments are unable to isolate a single property to measure. In many cases, sophisticated mechanistic models should be used together with the results of several experiments, in order to extract properties that are more fundamental.

2.6 On-line process control and optimization

The best way to optimize many processes is to control some aspect of them on-line. This requires a simple model, which correctly identifies the key parameters of the process and quantifies how they affect the product. Developing an on-line model and implementing it to control a process is the ultimate reason to model and is discussed in further detail in a later section.

2.7 Technology transfer

Finally, models also act as a means of technology transfer, which can be embedded in expert systems. An expert system can provide easy access to relatively complex models and a wealth of knowledge, without forcing the engineer to read and understand all of the literature.

Models are excellent educational tools. They enable visualization of the phenomena which control a process. The insights gained from careful evaluation of 3-D color moving images often cannot be obtained in any other way. Even the act of modeling can produce mental discipline in process analysis and deepen understanding of the phenomena which govern it. With increased process understanding, a process engineer can make better decisions and implement improvements to processes.

3. TYPES OF MODELS

All process models can be classified according to their empirical versus mechanistic basis.

A fully-empirical model is created by performing a curve-fitting procedure on the results of a statistical study with no attempt to understand the reasons for the relationships. This type of model is well-suited for online applications, because the resulting equations are very fast to solve, and robust, avoiding numerical difficulties. However, they usually become very inaccurate if extrapolated beyond the specific range of processing conditions for which they were developed.

A fully-mechanistic, or phenomenological, model solves equations based solely on the fundamental laws which govern natural phenomena. These laws include the differential equations governing the conservation and transport of mass, momentum, mechanical force, electromagnetic force and energy, in addition to thermodynamics, phase equilibria, kinetics, and other relations. Experimental data are incorporated in their most fundamental form, through the material properties. A mechanistic process model can be extended to understand and solve problems with a given process, without knowing the problem particulars prior to development of the model.

In practice, all models lie somewhere between these two extremes. No model comes close to being a complete, fully-mechanistic process model, despite the claims of some modelers. In reality, it is possible at best to model mechanistically only a tiny fraction of the actual phenomena present in a real process. This is because real industrial processes contain staggering complexities in phenomena at the mechanistic level. The continuous casting process, for example, is governed in part by the following phenomena:

- fully-turbulent, transient fluid motion in a complex geometry (inlet nozzle and strand liquid pool), affected by argon gas bubbles, thermal and solutal buoyancies
- thermodynamic reactions within and between the powder and steel phases
- flow and heat transport within the liquid and solid flux layers, which float on the top surface of the steel
- dynamic motion of the free liquid surfaces and interfaces, including the effects of surface tension, oscillation and gravity-induced waves, and flow in several phases
- transport of superheat through the turbulent molten steel
- transport of solute (including intermixing during a grade change)
- transport of complex-geometry inclusions through the liquid, including the effects of buoyancy, turbulent interactions, and possible entrapment of the inclusions on nozzle walls, gas bubbles, solidifying steel walls, and the top surface
- thermal, fluid, and mechanical interactions in the meniscus region between the solidifying meniscus, solid slag rim, infiltrating molten flux, liquid steel, powder layers, and inclusion particles.
- heat transport through the solidifying steel shell, the interface between shell and mold, (which contains powder layers and growing air gaps) and the copper mold.
- mass transport of powder down the gap between shell and mold
- distortion and wear of the mold walls and support rolls
- nucleation of solid crystals, both in the melt and against mold walls
- solidification of the steel shell, including the growth of grains and microstructures, phase transformations, precipitate formation, and microsegregation
- shrinkage of the solidifying steel shell, due to thermal contraction, phase transformations, and internal stresses
- stress generation within the solidifying steel shell, due to external forces, (mold friction, bulging between the support rolls, withdrawal, gravity) thermal strains, creep, and plasticity (which varies with temperature, grade, and cooling rate)
- crack formation
- coupled segregation, on both microscopic and macroscopic scales

For an arbitrary problem, any of these phenomena might be critical. Alternatively, the critical phenomena may not yet be identified. Finally, many of the fundamental material properties needed for such a mechanistic model are not yet understood, let alone measured.

Because of this overwhelming complexity, it is unlikely that any model will ever incorporate all of these phenomena mechanistically - nor should one! - the model would be too complex to ever run. All useful models focus on a specific aspect of a process, and mechanistically model only those phenomena most important to that aspect. Other phenomena are either ignored or incorporated empirically. Most models thus contain a significant component of empiricism. The great advantage of mechanistic models is that they can be extrapolated to simulate conditions outside the range of model validation. This makes them useful for design purposes.

Empirically-based models are sometimes looked down upon because they are inflexible and serve only a particular purpose. However, empirical models are ideally suited to online applications, which are so useful to industry. It is not necessary to achieve full understanding of an existing process before a model can be implemented. The unknowns can be accounted for in the empirical constants. Naturally, the better the understanding, the better the model will be. The challenge is to base the process model on mechanistic understanding, without sacrificing speed, simplicity, and robustness.

4. OTHER PROCESS DEVELOPMENT TOOLS

As already indicated, mathematical modeling is rarely sufficient, by itself as a mathematical exercise, to analyze the key characteristics of a materials process. Usually, some phenomena, such as the heat flux boundary conditions from a continuously cast strand to the water sprays, are poorly understood and are best treated using measurements. Many thermophysical properties, constitutive behavior, microstructural phenomena, rheological properties, or thermochemistry, have not been quantified and demand determination to build a credible model. Moreover, a process model that has not been tested with measurements can be a most dangerous distraction with the potential to inflict harm to process development.

Consequently, the application of mathematical models to the analysis and design of materials processes must always be set in the context of all of the other tools of process development. These other tools specifically include measurements, which may be conducted in at least four different realms: the real process, pilot plants, physical models, and the laboratory.

4.1 Industry experiments

On an operating process, by definition in the real world of complexity, measurements are obtained only with difficulty, especially in a production environment where pressures to meet schedules are severe and dominant. Commercial materials processes impose difficulties of noise, heat, dust, electrical interference, time, and space constraints. The frustrations of integrating a research program into the production environment are not insignificant, and are sometimes overwhelming; but the rewards, in terms of obtaining real world data, can be awesome. Much of what we have learned from processes like continuous casting, copper converting and zinc slag fuming wells up from difficult, time-consuming, and often stressful measurements made on the operating process. Such experiments probe the complexity of fluid interaction, heat flow, and chemical reactions which are not easily replicated under laboratory conditions.

4.2 Pilot plant experiments

That having been said, the pilot plant, which is a smaller scale of a potential or operating process, can be a powerful tool of process development. The pilot plant affords the opportunity to study, away from the pressures of the production environment, the influence of process parameters on the production rate, quality, safety, and operational care, amongst others, on the process operation. The size of the pilot plant may vary from laboratory (bench) scale to a larger size, but the goal always is to understand, assess and develop a process at reduced capital cost which minimizes financial risk.

4.3 Physical model experiments

The physical model is another tool of process analysis which is aimed at simulating some of the phenomena of a new, or existing, process through the use of more user-friendly systems, like Plexiglas and water, as compared to molten steel and refractory. Physical models have been employed most frequently to study fluid flow in vessels, such as continuous casting tundishes, where the relevant properties of water and molten metal are similar. In the design of physical models, similarity criteria need to be considered so that the forces at work in the real process are simulated properly. Such forces in fluid flow include inertial, viscous, buoyancy, and surface tension, which may be characterized by the Reynolds, Froude, and Weber numbers. It is critical that the dominant forces in a process are evaluated because it is rare that all similarity criteria can be met with the physical model. For example, a hot metallurgical processes is accurately simulated with a cold isothermal liquid only when the buoyancy forces are small, as indicated by the size of the modified Froude number. Physical models can be applied to measure mixing conditions, or with the help of sophisticated tools like the laser Doppler velocimeter, turbulence in the fluid. The scaling and use of physical models must be undertaken with considerable forethought and ingenuity, but they can yield important results on complex metals processes at relatively low cost.

4.4 Laboratory experiments

Finally, the process engineer has in his arsenal, measurements in the laboratory. Measurements in a carefully-controlled laboratory setting may range from determination of thermodynamic activities, to the rate of the Boudouard (C-CO_2) reaction, to the study of sulfide particle disintegration in a flash smelting environment.

It cannot be over-emphasized that, in the modeling of complex processes, mathematics can take us only so far. When inevitably we hit the wall of our understanding, measurements must be made. All too frequently, the modeller takes the easy route of making simplifying assumptions to skirt the difficulty and remain at the computer keyboard, rather than move to the laboratory. This is a mistake. Properly formulated, a mathematical model automatically guides us to what we must know, in terms of properties and boundary conditions. What is missing must be measured. Mathematical modeling is often more about measurement than it is about mathematics. A wise process modeller uses all of his tools, including process models, to develop and improve materials processes.

5. DEVELOPMENT OF A PROCESS MODEL

The process of developing a process model can be divided into several stages, which are illustrated in Figure 8.2. In practice, models evolve as understanding improves, so there is cycling between the various steps.

5.1 Problem definition.

As in any other endeavor, success in modeling is more likely when there are clear objectives. When developing, applying, evaluating, and implementing a model, a multitude of decisions must be made, such as the choice of phenomena to simplify or ignore. Each decision should be made by considering the exact purpose of the model, or what problem in the real world the model is intended to help solve. Defining the specific reason for the model is the most important step in model development.

5.2 Identify key phenomena

An initial goal of the process engineer in developing a process is to identify the rate limiting steps and to determine how to control, accelerate, or optimize them. The same is true of the process model.

Before developing a process model, it is essential to have a qualitative understanding of the basic phenomena which govern the process. This is because models, at best, can only quantify that understanding and shed insight into the interactions between those chosen phenomena. A model cannot identify phenomena which have been neglected. Important phenomena which are poorly understood, particularly those occurring at the boundaries, are often best treated empirically by calibrating the model with experimental measurements.

To choose the phenomena to model mechanistically, the modeller should bring in as much process understanding as possible from all other available sources. The place to start is with previous literature and experience. This includes the insights from previous laboratory, pilot-plant, and industry experiments, physical and mathematical models, discussed in the previous section. Simple “back-of-the-envelope” calculations and analytical solutions are invaluable as well. Scaling calculations are a crude preliminary tool to eliminate phenomena that are unimportant.

It is critical to identify the key phenomena or rate-limiting steps which govern the process correctly. Input from all process analysis tools should be gathered together and carefully evaluated, before making the choices for this critical stage of model development.

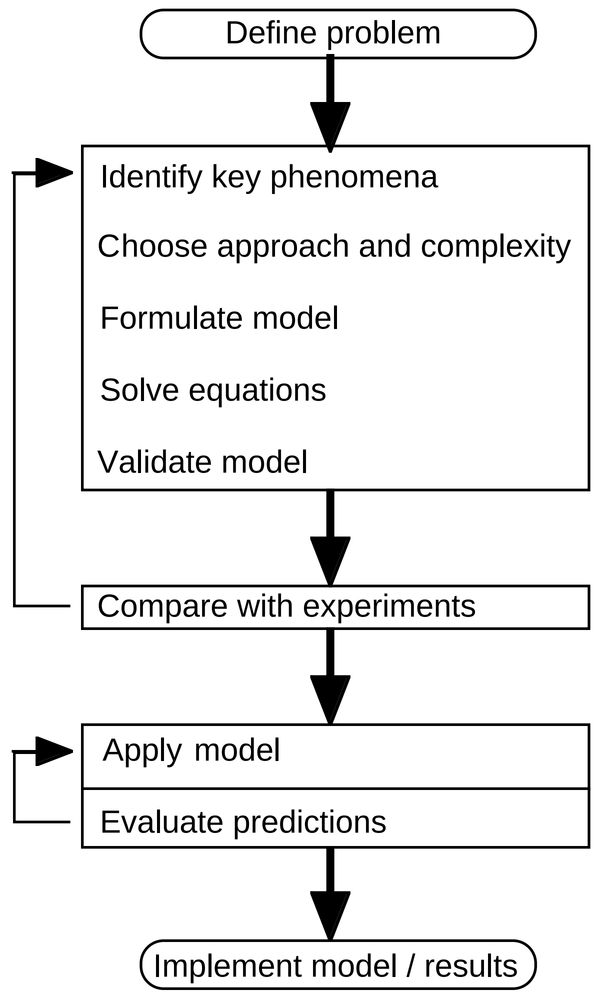

Figure 8.2. Steps in process modeling

5.3 Approach and Model Complexity

Next, the type and complexity of the model must be chosen. Process models range in complexity from simple analytical solutions to fully-coupled, three-dimensional transient numerical simulations. Including another phenomenon often adds another dependent variable, (such as concentration, temperature, velocity / pressure, or displacement), or another material property. The purpose of the model should dictate what phenomena are included, and consequently how complex the model should be.

The first guideline is to choose the overall model complexity according to the computing hardware power and time frame available. A common mistake is over-complexity. Models for eventual online use must be kept simple, to run in minutes or less on small computers. Other models can afford to include more mechanistic phenomena, and consequently be more complex. Even then, the developer should consider that a model which requires several weeks of execution time per run on a supercomputer is unlikely to be productive, although it is surprisingly easy for this to happen.

The next guideline is to model phenomena in proportion both to their importance to the problem and to how well they are understood mechanistically. Important phenomena, which are well-understood, are worthy of modeling in detail. For example, detailed simulation of heat conduction in a complex geometry has been the basis of many successful models. Phenomena which are not well understood are best left to simple empirical approximations, based on experiments. For example, convection heat transfer between spray water droplets and a hot surface is generally best modeled empirically using correlations from experimental data: heat transfer coefficients.

Another guideline is to keep the relative errors about the same. There is no sense in modeling one aspect of the process (such as the geometric effect of the third dimension) to gain a 1% improvement in accuracy, while at the same time making a 100% error by ignoring another critical aspect of the process altogether, (such as transient effects, or upstream process variations).

All process models should aim to simulate phenomena in the real world, which is always three-dimensional. To do this, it is sometimes necessary to discretize all three dimensions, thus producing a “3-D model”. Often, however, it is possible to make reasonable approximations, which avoid discretizing one or more of the dimensions. This allows huge computational savings, because in general, each dimension discretized increases the complexity of a model by an order of magnitude. Before including that third dimension, it is logical to ensure that no other important phenomena are left out of the model. It is often easier to improve the accuracy of a model by a crude incorporation of some secondary phenomena than by an exact modeling of the primary phenomena in three dimensions.

A process model should be kept as simple as possible, but no simpler! Overly complex models are too difficult and time consuming to run. On the other hand, simplifications which are not reasonable may lead to erroneous conclusions that may be very costly. Thus, it is impossible to create an efficient model of sufficient accuracy without knowing how the model will be used. Granted, this is a difficult task.

5.4 Model Formulation

Formulation of the mathematical equations to solve is often the least difficult of the stages in model development. Naturally, this depends on the complexity of the phenomena to be modeled and on the availability of commercial software packages which can drastically reduce the time to develop a model. More is said about commercial software in the next section, but these packages should not be used without a sound understanding of the principles and assumptions which underpin them.

An essential aspect of model formulation is the making of assumptions which, if done properly, enable us to model the important phenomena more easily, and with minimal loss of accuracy. What to assume requires a careful assessment of the process, as described earlier, and good judgment. The wrong assumptions cause us to ignore important phenomena. Too many assumptions oversimplify the model, ultimately leading to greater empiricism and less flexibility.

Too few assumptions may over-complexify a model and create needless expenditure of time and money for no tangible gain. Clearly, the ability to formulate the best assumptions can place the mathematical model on track toward process development, or seriously de-rail it.

A mathematical model rooted in fundamental laws and mechanisms must conform to the laws of conservation of mass, heat, energy, and momentum. In order to apply conservation, a part of the system must be isolated; and thus a volume element must be defined. This volume element may represent a significant portion of the system, leading to global balance equations. Such could be the case for thermodynamic models or reactor models. Alternatively, the volume element may have small or even infinitesimal dimensions in one, two, or three different coordinate directions, depending on the number of dimensions chosen for the model. The choice involves a balance between model simplicity and potential accuracy, as already discussed.

Having defined the volume element, a balance is performed on the quantity to be conserved, (mass, heat, momentum):

Input through surfaces of volume element + Generation within element volume

= Output through surfaces of volume element + Consumption within volume element + Net accumulation within volume element

These balance equations yield the governing equations, which relate the dependent variables to the independent variables of space and time. In the case of a mass balance, the dependent variable is concentration. The heat balance yields temperature, and the momentum / mass balance yields velocity and pressure as dependent variables.

The equations can be built directly into "finite volume" models, by constructing an algebraic equation for each volume element. Alternatively, a partial differential equation form of the balance can be written based on infinitesimal volume elements, and the discrete system of simultaneous algebraic equations derived using any of a variety of mathematical techniques, such as the Galerkin finite element method (Zienkiewicz and Taylor, 1988)

The final step in the mathematical formulation is the specification of initial and / or boundary conditions subject to which the governing equations are solved. Specifying a particular boundary condition depends on the phenomena occurring at that boundary and is usually relatively straight forward. Determining the coefficients, such as for heat and mass transfer, that appear in the boundary conditions is much more difficult. For most processes, the Handbooks do not contain all of the information we need. In the absence of previous published data on a relevant system, measurements are required, as described earlier. An otherwise well-formulated process model, with the wrong boundary condition coefficients, will yield wrong predictions. The same can be said for the coefficients in the governing equations and initial conditions.

Further details on the equations for modeling specific phenomena are described in other chapters. These include thermodynamic models in Chapter 3, mass balance and reactor models in Chapter 9, fluid flow models in Chapter 7, and heat transfer with solidification in Chapters 6 and 12.

5.5 Solution

Next the model equations must be solved, generally by computer. For models which do not have to run online, it is often easiest to employ a general-purpose, commercial software package to do this, as many powerful programs are now available. These include flow sheet programs, such as METSIM (Bartlett, 1996) for the construction and solution of global balance equations for chemical reactions, based on global balances of mass and heat. These programs include thermodynamic databases and have been used successfully to model both metallurgical and chemical processes, as described in other chapters. Software specifically for thermodynamic calculations includes FACT (Thompson, 1996) and THERMO-CALC (Sundman, 1993).

Fluid flow, including 3-D turbulent behavior, can be solved using any of dozens of programs. In complex geometries, finite element software, such as FIDAP (Engleman, 1994), has been used successfully (Najjar et. al., 1995). For simpler geometries, finite difference software, such as FLUENT (1996) may be more computationally efficient. For stress analysis, packages such as ABAQUS (1994) include powerful algorithms for integration of the non-linear constitutive equations that characterize most materials processes. Most of the fluid flow and stress analysis software can also simulate heat transfer, including complex phenomena such as solidification. These packages offer convenient user interfaces to input choices which define the model equations, material property data, and boundary conditions. Evaluation of results is aided by powerful post processing abilities built into most packages, such as color movies of contour plots of the solution variables.

It must be emphasized that commercial packages have difficulty solving the complex equations which are most relevant to real processes, even when features to model the desired phenomena are provided. For example, numerical problems are often encountered when simulating multiphase turbulent flow or free-surface movement with current fluid flow programs.

As an alternative to commercial packages, it may be better to develop a special-purpose program to model particular aspects of a specific process. This enables unique features and a faster program which is easier to use. Examples for the process of continuous casting of steel slabs include CON1D (Thomas et. al., 1992) for heat transfer in the mold, and MIX1D (Thomas and Huang, 1994) for intermixing during a grade change. Sometimes, it is convenient to use commercial packages to display the results of a special purpose program. Software specifically designed for this task includes TEKPLOT (1996) for viewing 3-D flow results on a regular grid and GNUPLOT (Williams and Kelley, 1996) for fast, simple 2-D graphs on a variety of hardware.

5.6 Model Validation

Comparison of the model predictions with known solutions is an important step in model development to verify numerical integrity of the model, for all of its conceivable uses. The test problem(s) should be chosen such that the model is theoretically capable of an exact match with the known solution. Then, the values of numerical parameters (such as mesh and time step size) required to achieve acceptable accuracy can be clearly identified. To be most useful, the test problem should match the process phenomena and conditions of interest as closely as possible. This stage in model development is particularly important for self-developed codes, to ensure there are no programming errors. Testing of models based on commercial packages also verifies that they are being used correctly. Finally, this stage of model building also can provide early insights into the results, if the test problem is chosen carefully.

Test problems generally must be simple. When validating the model during this stage, however, it is best to use a test problem that invokes as many of the features of the ultimate model as possible. For example, to validate a 3-D finite-element model using a 1-D test problem, it is best to use a single row of 3-D elements. Even better is to simulate an axisymmetric test problem with a Cartesian numerical grid. In this way, a 1-D solution can validate a 2-D numerical scheme. Often, several different test problems are needed to validate all of the features of a process model.

5.7 Comparison with Experiments

Comparison of model predictions with experiments is a critical phase of using a model, once its internal numerical consistency has been verified. Important knowledge is always gained, regardless of whether or not there is a match! If the results *do* match experimental observations and measurements, then there is strong circumstantial evidence that the both the model and the experiments are correct. This implies that the correct phenomena have been modeled, the assumptions are reasonable, and the constants are valid, to the extent of the match. Of course, it is always possible for a coincidental cancellation of errors, which must be carefully guarded against by comparing with as many experiments as possible.

If the model predictions do not match the experimental measurements, then something is wrong with either the model, its input data, or the experiments themselves. In every case, there is an opportunity to learn something.

Sometimes, it is possible to identify a phenomenon which is responsible for the mismatch. If this phenomenon can be accounted for quantitatively in the model by changing only a few parameters, then the model can be "calibrated" to the experiments by choosing value(s) for the parameter(s) that make the model achieve the match.

Consider, for example, an online 1-D heat conduction model of continuous casting to trouble-shoot the origin of cracks, which form at the solidification front, and to optimize cooling water flow rates in the spray zone. The heat transfer coefficients may be obtained as a function of water flow rate using careful laboratory experiments. Suppose that validation of this model using plant data reveals that the model overpredicts the "metallurgical length" of the strand, which is the distance below the top of the mold where the steel first becomes fully solid. Further comparison with a 3-D version of the model on a super computer yields similar results, proving that the 1-D assumption is not the problem. (This could also have been shown through simple scaling calculations.) The problem with this model is neglecting the tremendous enhancement in heat transfer through the liquid phase which is produced by the turbulent flow inside the solidifying steel strand. Considering the purpose of this model, it is unjustified to include a mechanistic treatment of the liquid phase, even though this could be done. Instead, the "effective" thermal conductivity of the liquid can be increased until the model predictions match the experiments. The resulting "calibrated" model can be implemented at the caster to make reliable, quantitative predictions to avoid cracks. For its intended purpose, this crude, but calibrated, model is far superior to a fully-coupled model of turbulent flow, heat transfer and solidification, which would be too slow and complex to run at the caster.

Another possibility, if experiments and model predictions do not match, is that one (or more) of the model assumptions is wrong. For example, when attempting to use a coupled thermal-stress model (as an off-line literature model) to simulate the formation of particular surface shape defect, it was found to be impossible to match any of the facts known about the defect through plant experiments. Checking all of the model assumptions, the only one that seemed highly questionable was the assumption of uniform heat extraction. The model was therefore improved to vary heat extraction by accounting for the lower heat flow across wider interfacial gaps. It was then possible to match the experimental trends (Moitra and Thomas, 1993). Furthermore, the original simulation suggested that the defect might be avoided by finding a means to make the heat extraction more uniform. This example is intended to show that hypothesis testing using the model together with experimental measurements is a good way to gain insight.

Finally, when comparing with experiments, it is important to model the experiment exactly. Even though the experiment might not match the process as intended, it is still of value to model validation, so long as the conditions and results were measured accurately. For example, the steel shell thickness predicted by a solidification model of the continuously-cast strand might not match that measured from a "breakout shell". This could be due to conditions unique to the breakout, such as the extra solidification during the time taken for the molten steel to drain from the hole in the shell. Proper accounting of special effects such as these could enable the model predictions to match the breakout shell (Moitra and Thomas, 1993). Appropriate changes would be made for subsequent use of the model to simulate standard casting conditions. Every experiment has its own potential pitfalls, which should be investigated carefully.

6. MODEL IMPLEMENTATION

Hopefully, a better understanding of how models are implemented in practice will lead to more effective model implementation and avoid the all-too-common waste of models that are never implemented. The ultimate goal is not to model, but to develop a process.

6.1 Definition of model implementation.

A model has been "implemented" only after the modeling exercise has led to some tangible change in the process, which ultimately benefits the industry.

To understand this definition, it must be recognized that the principal aim of industry is to make a profit. In materials-processing based industries, two possible ways to help do this is are to improve product quality and to reduce production cost.

One way to improve quality is to eliminate defects. Thus, a reasonable objective for a process model could be to eliminate some defect by specifying achievable changes in the process. Note the two key terms: "eliminate" the defect and "achievable" changes.

Many process modeling efforts aim to predict the occurrence of some kind of defect, such as segregation or impurities in the product. These models may provide valuable insight into the phenomena that underlie the formation of the defect. Before it is truly useful, however, this phenomenological understanding, which is often gained only by the modeller, must be translated into beneficial process changes, such as actually eliminating the defect.

The second point is that process changes need to be achievable. Thus, models should first identify input and output variables that can be changed in the plant. Another pitfall to avoid is running the model for conditions which are infeasible to achieve in practice. If the model is too complex for anyone else to rerun, then the potential implementation has been lost.

Changes to the plant process can be classified according to the time needed to effect them. "Design variables" are relatively difficult and time-consuming to change. Standard operating practice, or "SOP" variables, refer to the set points of process variables that are relatively easy to change. "Control variables" change rapidly with time, to accommodate variations in input conditions (both accidental and intentional) and customer demands on the product.

In continuous casting, for example, mold geometry and roll spacing are design variables, which require major, expensive plant reconstruction to change. SOP variables include mold water flow rate and tundish level, which are set to desired levels. Slide gate opening position is a control variable that changes continuously to maintain a constant liquid level in the mold. Depending on the availability of online models, some variables, such as casting speed, can either be set at SOP levels, or controlled to adapt to variations in the process, (such as slowing down casting speed temporarily to avoid an impending breakout disaster). Upgrading SOP variables to control variables has obvious advantages for improving the process operation.

For a model to have any impact in industry, it must be implemented. The above definition of model implementation requires that changes take place in the plant. If nothing ever changes as a result of the modeling, then the entire exercise was wasted. This reasonable definition sets a demanding context for the evaluation of most models reported in the literature. The rest of this section explores how process models are implemented according to this definition, and to comment on the implications for process modelers.

6.2 Ways to implement a model

There are many paths to model implementation, illustrated in Figure 8.3. Process models are classified here according to how their results are implemented into practical process changes:

- fully-online models
- semi-online models
- off-line models
- literature models

Online models implement beneficial change in the plant directly. Offline and literature models contribute to process understanding, leading to implementation by others. Semi-online models lie somewhere in between. The next sections further define and examine how each type of model is implemented, in order of its immediate impact in industry.

6.3 Fully-online models

Fully-online models are part of the computer system controlling the process at the plant. They obtain their input data directly from the system (which has access to the relevant sensor signals) and make direct changes to specific control variables, possibly under the supervision of an operator. Fully-online models represent the pinnacle of model implementation, as the model itself implements change in the plant on a continuous basis.

For example, the spray water system on a slab casting machine is generally controlled by a fully-online model. The model is typically designed to deliver the same total amount of water to each portion of the strand surface, changing the flow rate to account for variations in the casting speed history experienced by each portion as it passes through the spray zones.

Another example is a breakout detection system, which predicts when there is danger of a "breakout", (where molten steel escapes the solidifying shell and drains over the lower portion of the continuous casting machine) and slows down the casting withdrawal speed to prevent this from happening. The model continuously analyzes the temperature signals from thermocouples embedded throughout the mold and searches for patterns, such as low total heat flux (Gilles, 1981), or moving temperature inversions (Itoyama, 1988), that are associated with an impending breakout.

Fully-online models must be extremely fast (to run in real time) and robust (to produce reasonable output for any input condition, including signals from bad sensors) These needs require that the model be extremely simple, consisting only of logic and a few basic equations, that have been thoroughly tested to be reliable.

The demands for reliable accuracy are higher for online models than for any other type of model. To meet this need first requires detailed knowledge and understanding of that aspect of the process being controlled. If the model is designed to prevent a defect, for example, then the exact nature of the formation of the defect must first be understood. In the case of breakout detection systems, for example, the relationship between thermocouple signals and the unusual sequence of events that accompanies solidification prior to a sticker breakout has been determined through extensive plant and pilot-plant experimentation (Gilles, 1981), (Itoyama, 1988).

In addition to containing an accurate qualitative understanding, the model must also be quantitative. This generally requires extensive calibration at the particular plant in question. In the context of our example, the actual magnitude of the critical temperature inversion must be built into the model, or else the breakout detection system could generate costly false alarms (if the model value was too low) or allow breakouts (if the value was too high).

Generating the knowledge needed, and refining it into a few simple equations, is the most demanding part of fully-online model development. Fortunately, the model need only produce accurate results for the limited set of process conditions at a particular plant. Therefore, the equations may be based on curve-fits of the results from plant, pilot-plant, physical model, or laboratory-scale measurements, or even sophisticated numerical experiments. Optimization methods such as neural networks provide a useful tool for this task (Middle and Khalaf, 1995). In each way, the fundamental knowledge is incorporated into simple empirical relations and constants.

Implementing the model into the plant requires extensive work to install and maintain sensors, data acquisition, and interfacing computer systems to link the process with the computer model. This is a very time-consuming and expensive undertaking, so it is critical that the model is sufficiently beneficial, accurate and robust to be worth the trouble.

Fully-online models deal with control variables, by definition. These models transform an SOP variable into a control variable, enabling significant process improvement. With better process understanding, more SOP variables can be transformed into control variables, through the use of fully-online models. This enables savings in operator time, improved productivity, and product quality by adapting faster and more consistently to changing process conditions. Universities can contribute to this effort by helping to develop the understanding and simple basic principles that form the heart of these models. In this regard, intelligent control systems, such as the intelligent mold (Brimacombe, 1993), have great potential benefit to industry, as fully-online models of the future.

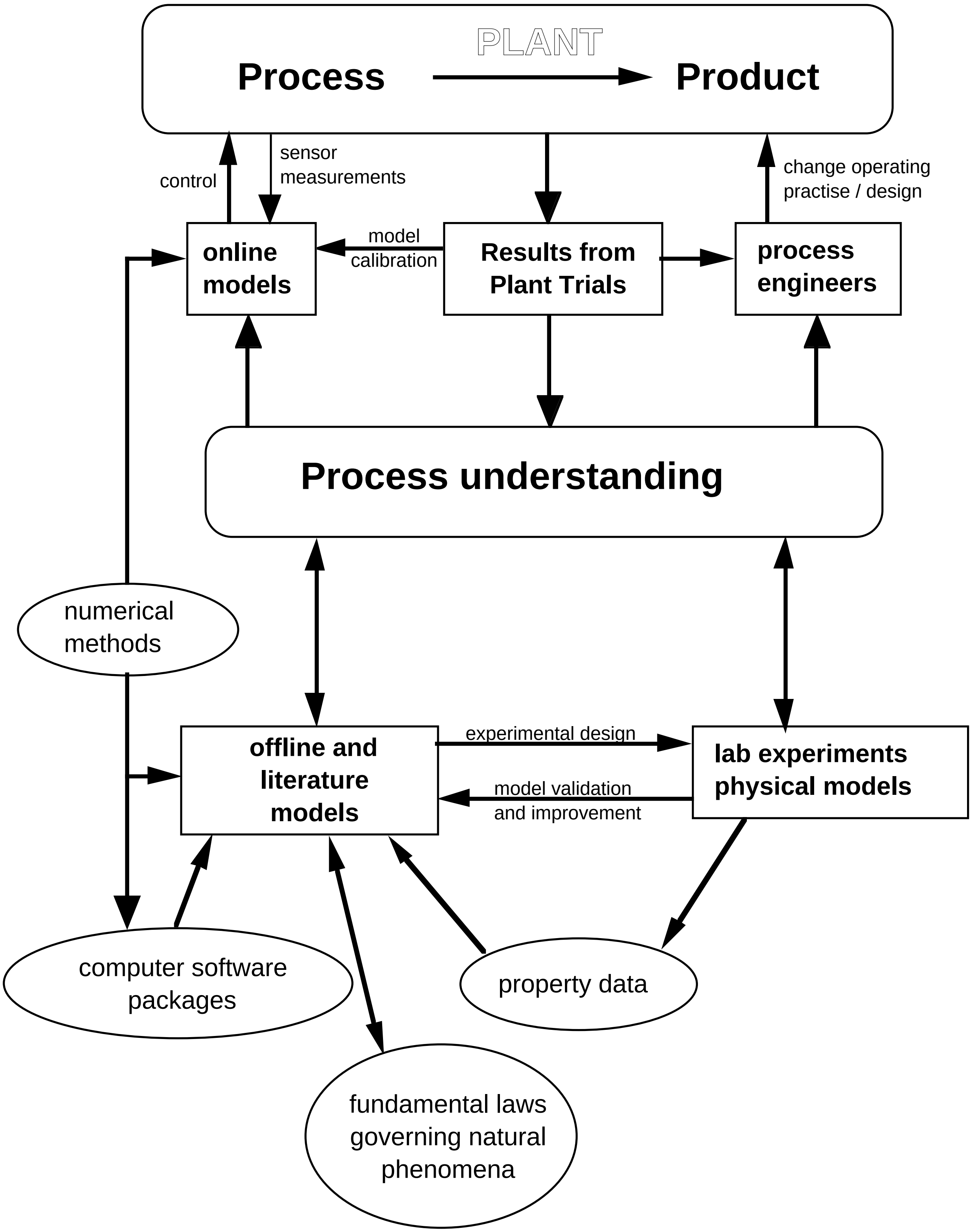

Figure 8.3. Flow chart for the implementation of process models in industry

6.4 Semi-online models

Semi-online models are similar to fully-online models, except that a plant operator or process engineer interfaces between the model and the process to determine what action to take. This is an important distinction in practice, which affects the nature of model implementation and the features required of the model. These models are best suited to help set optimum levels for SOP variables, which need less frequent change than control variables.

A typical semi-online model runs on a stand-alone personal computer on the operator's desk. For example, in a continuous casting process, such a model might be used to indicate the optimum places to cut the strand during a grade change, in order to minimize the amount of intermixed steel that must be downgraded (Thomas and Huang, 1994). Each time a new ladle is tapped that involves a grade change, the operator inputs the relevant current process conditions and grade specification limits for that customer, runs the model, and interprets the output to decide where to cut the strand.

A semi-online model could also act as a tool for trouble-shooting and on-the-spot problem solving. For example, a fully-calibrated, 1-D heat-transfer model of a continuous slab caster could be used to determine which rolls to change or realign in order to solve certain types of cracking problems. It does this by calculating the shell thickness as a function of distance down the strand. Misaligned or worn rolls can generate certain types of internal cracks by straining the weak solid at the solidification front. The initiation point of these cracks, measured on a sectioned sample of the slab, corresponds to the location of the solidification front at the time the crack was formed. For this model to be effective, it must be calibrated for the different grades and casting conditions at that plant. In addition, the operator must have access to the metallurgical results and knowledge about the cracks. More advanced semi-online models, such as the expert system of billet casting developed by Brimacombe and coworkers (Brimacombe, 1993), make this analysis even easier, and supply useful knowledge to solve other types of problems as well.

Sometimes, a good, well-calibrated model can be implemented in more than one way. For example, the 1-D heat conduction model just discussed, could also be applied to optimize cooling water flow rates in the spray zone of the continuous slab casting machine, in order to achieve a desired temperature history for the steel surface, and thereby avoid surface cracks.

Semi-online models have many attributes that are similar to fully-online models. Both must run very quickly (a decision is often needed within a minute) and make quantitatively-accurate predictions, thus requiring extensive model calibration at the plant. In both cases, the potential benefits from the model are controlled by the extent to which the phenomena governing the process are understood and properly quantified in the model.

In comparison with fully-online models, semi-online models are better suited to modeling complex phenomena. This is because the operator can respond to information and circumstances unforeseen by the model to make a better decision. It is also easier for the operator to learn from the semi-online model, which serves as a valuable means of technology transfer between the model developer and the plant operator. The semi-online model requires substantially less effort to implement into the plant, as less computer automation and interfacing systems are needed. It is consequently much easier to change the model, to modify or add new knowledge and capabilities.

An important feature of semi-online models is that they must be easy to run and have a very "user-friendly" interface with the operator. Developing this interface is one of the difficult tasks which separates these models from all others. Semi-online models which prove to be worthy might eventually be implemented as fully-online models. The semi-online stage provides the opportunity to learn about the process, and optimize the model, by determining all of the essential minimum number of input variables, in addition to refining its accuracy and robustness.

6.5 Off-line models

Off-line models are used by process engineers and designers (in the plant, research, quality control, etc.) to gain personal insights and understanding about a process. The model results are then implemented in the plant by developing new designs or changes to standard operating practices. These models are not as immediately beneficial as online models, because off-line models at best can only help to prevent a problem from occurring the *next* time. More importantly, model implementation relies solely on the model user.

To implement beneficial changes, the user of an off-line model must have a thorough understanding of both the process and the model. The model developer should make it clear (through the user manual) what the model assumptions are. To generate the process understanding, Figure 8.3 illustrates how the off-line model is just one of the tools that can be used. Model results are implemented in combination with the user's personal knowledge, obtained from plant, pilot-plant, physical model, and laboratory experiments, previous literature, and other sources.

As shown in Figure 8.3, the process understanding gained from all of these sources can help a process engineer to implement positive changes in the plant. This can help to avoid the dangerous short cut, also shown in Figure 8.3, of implementing changes in the plant on the basis of trial results without understanding the process.

Off-line models can help to provide insights in many different ways. They can correct misconceptions about the process, by quantifying phenomena (such as internal temperature and flow patterns) which the process engineer has never seen or measured. The model can also be used for hypothesis testing, by putting numbers on a hand waving argument. For example, a qualitative mechanism may be suggested to explain some observed event in the plant. A process model could quantify the mechanism, which can then be reevaluated based on how closely the model results match the expected behavior.

Generally, the next stage of implementation is to design plant trials to test the expected improvements. Off-line models can help in this experimental design. They are most useful when the plant trials are very expensive. This is certainly the case when developing a new process. Tracking the effect of a process change on the incidence of a defect in an existing process may also be expensive. This is because it is usually impossible to control plant experiments very well, so the results are statistical, which demands long trials before a conclusion can be made with confidence. Off-line models are also important to understanding the results of plant trials.

Another stage of implementation is finding the "optimum" way to run the process to save money. Parametric studies or "numerical experiments" with an off-line model can play an important role in this regard. For example, the model of intermixing during a grade change discussed previously could be used off-line to investigate how to minimize the amount of downgraded steel created. The process engineer could learn by running the model that draining the tundish to a low level before opening the ladle and decreasing the casting speed during the grade change would shorten the downgraded length. Further investigation would be required to determine if the slowdown in production to save this amount of downgrading is cost effective. If beneficial, the new practice could be implemented in the plant through changes in the standard operating practice.

Off-line models should be easy to use, leaving time for the user to pursue insights using other tools and to implement the results. Rapid turn-around time between model runs is also important to attain the immediacy needed to understand the behavior of the model. Although commercial packages are the most popular framework for offline models, they only barely satisfy these requirements. If a process model is too difficult to use, it may be easier to obtain the needed knowledge another way, such as through experiments, or even trial and error in the plant.

To help implement changes, off-line models must be able to simulate process situations outside the scope of prior experience. Thus, the model should be as mechanistic as possible, with its roots grounded solidly in fundamental principles, as illustrated in Figure 8.3. Properly incorporating the phenomena which govern that aspect of the process being modeled, allows the model to make reasonable predictions for new conditions. This enables implementation of new designs and radical changes in operating conditions. It also makes model validation and calibration with experiments easier.

Unfortunately, the same sophistication that enables off-line advances in understanding also tends to complicate and slow down the model. This makes the model difficult to use online. Sometimes, a simplified version of an off-line model can be developed for online use later.

6.6 Literature models

Literature models are defined here as off-line models which are used only by the person(s) who developed the model. Furthermore, the modeller has no direct contact with the process, (working generally in a University or research environment). The only direct way for these models to be implemented (if they are implemented at all!) is by someone else using the reported results.

At their best, literature models can act as off-line models, possibly saving a process engineer time in developing and running a very complex model. Moreover, the literature model can afford the luxury of long computing times, (even a week on a supercomputer), so may include more of the phenomena which govern the process.

Like the off-line model, the knowledge and insights gained by the process engineer are more important than the model itself. It is therefore important that conclusions from the model be communicated clearly. The more practical and specific the insights, the easier for implementation. It is perfectly reasonable to combine the modeling results with experimental results, physical models, and plant data, perhaps found in existing literature. The aim is to present as complete an understanding as possible to the person reading the paper. Ideally, the process engineer can search the literature, to learn how to solve his specific problem, and implement a course of action in the plant, in a similar manner to a doctor diagnosing and treating a patient.

Because the modeller and user are the same person, significant short-cuts in developing the user interface of the model are permitted. Of course, this usually makes the model too complex and “user-vicious” for anyone else but the modeller to run.

A key attribute of the literature model is that there is no opportunity for the process engineer to rerun the model. All of the parametric studies must be done by the original author. For the results to be implemented, it is important that the modeller make reasonable assumptions regarding both the phenomena included in the model, and the input conditions adopted in parametric studies. To do this, the modeller must obtain a good understanding of the process.

The implementation value of a model is less when it merely echoes knowledge already known through plant experience or other means. Its value is negative when it contradicts some of that knowledge and fails to explain why. Particularly for well-established processes, there is a great deal of knowledge already in existence. To ensure a positive contribution to industry, this prior knowledge should be taken into account. Well-studied processes generally require more sophisticated models to contribute new knowledge than early models of a new process.

To be useful to industry, the results are best presented in the form recommended by Herbertson (1993) in Figure 8.4. In this figure, “you” refers to the process engineer, so ideally, the y axis should relate to some aspect of quality or productivity. The x axis should contain a design or operating variable which can be changed in the plant.

The modeller should avoid presenting results in terms of intermediate variables, which are difficult to control, or even measure, in practice. For example, it is natural to use a model to find the desired heat flux or heat transfer coefficient needed to optimize some aspect of a given process. This is not as useful as specifying the actual fluid flow rate needed to achieve this heat transfer condition for the specific process under consideration.

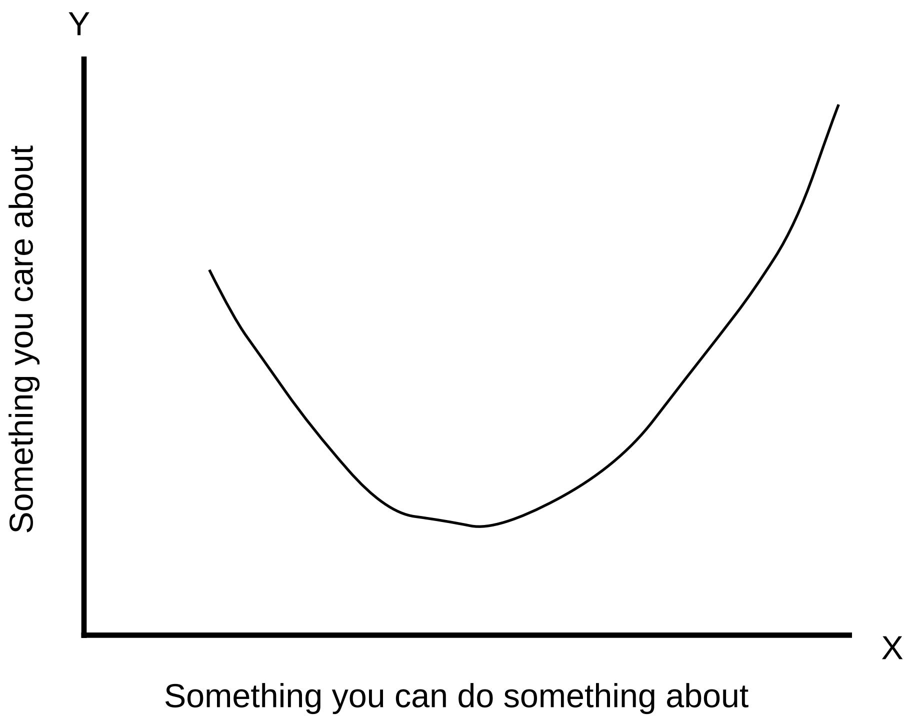

Figure 8.4. Graph containing results which can be implemented

The quality of presentation of the results is independent from their accuracy. Potential weaknesses of a model should be identified, in addition to its strong points. It is also useful to point out when the results are known to form upper or lower bounds to the true behavior. To increase the credibility of the entire modeling community, it is the responsibility of each modeller to continually strive for accurate modeling conclusions, by understanding the process of interest and validating the model.

7. SUMMARY

The rapid development of computer hardware and software over three decades has made the mathematical model a key component in process development. This chapter has presented some guidelines for the development and implementation of process models.

A successful model must have a purpose, which dictates how choices are made during its development. Reasons to model include increasing process understanding, helping with the design of experiments, evaluation of experimental results, scale-up, quantifying property measurement, online process control and optimization, and technology transfer.

Modeling must be accompanied by careful measurements as needed, whether they be made on an operating industrial process, a pilot plant, a physical model, or a laboratory apparatus. The process model must be viewed as one of the many tools of the process engineer, which also includes previous literature and experience.

Models are implemented when they lead to beneficial changes to plant operation. This is most likely when the model is explicitly targeted at understanding how particular design, process, or control parameters can be changed to affect specific quality or productivity variables. Models range in complexity from simple empirical models, suited for online implementation, to sophisticated mechanistic models, which can be used for in-depth offline analysis.

When properly formulated, process models can yield insights to process behavior that cannot be fathomed by other means, and lead to significant process improvements. However, when key phenomena are ignored, or predictions are carelessly analyzed, great harm can be done.

Successful modeling requires understanding of both the industrial process and the computer model. The process engineer has the responsibility to ensure that a process model adequately represents a system and interprets the results appropriately.

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