MATERIALS PROCESSING IN THE COMPUTER AGE

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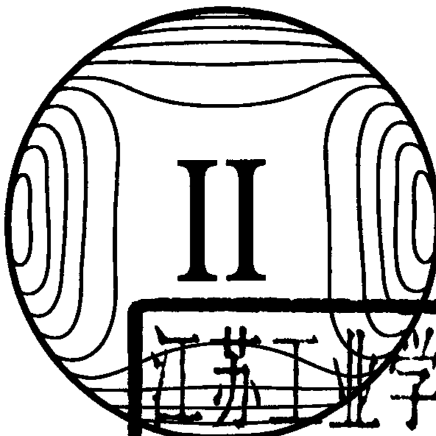

Proceedings of the 2nd International Symposium
Sponsored by TMS Synthesis, Control and Analysis
in Materials Processing Committee,
TMS Solidification Committee, and
TMS Process Fundamentals Committee

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PREFACE

The papers in this volume were presented at the 2nd International Symposium on Materials Processing in the Computer Age. The major objective of this series of Symposia is to address the question

What are the current and future roles of computer technology in the analysis of materials processing operations?

The first symposium took as It is theme the concept of a "computational laboratory"; an environment in which modelling and analysis leading to improved process understanding could be undertaken. This theme of modelling for understanding is still present in many of the contributions of the current proceedings. Complimenting this, however, is a strong emphasis on the use and application of models. This theme is very evident in the first two invited papers that consider, in turn, the role of process models in industry and the development of modelling software for the casting industry.

As with the previous volume in the series, a large group of contributed papers are directed at the modelling and analysis of solidification processes and phenomena. These works include the latest developments in macro scale modelling of heat and mass transfer, micro scale modelling of microstructure and the coupling of scales.

Another group of papers covers the important topic areas of physical modelling, measurement and control. This group includes an invited paper which clearly illustrates the benefits of physical modelling in gaining process insight. Contributed papers cover topics ranging from the design of space experiments through to the development of novel measurement and control strategies for materials processing operations.

The current volume is completed by a group of papers that discuss the role of computational approaches in the analysis of electromagnetic and emerging processes. There is a suite of contributed papers, from some of the leading researchers in the field, addressing problems associated with electrodynamic materials processing systems. Other papers in this group focus on emerging processes such as the manufacture of superconducting wires and polymer molding. The papers in this group also contain a strong numerical flavor and some contributions make worthwhile comparisons of the performance of various numerical methods.

Altogether the papers in the current volume are representative of the current sate of computational analysis in many areas of materials processing. On comparison with the previous symposium the papers also indicate a pleasing trend away from the computational laboratory and into the physical plant.

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INVITED PAPERS

COMMENTS ON THE INDUSTRIAL APPLICATION OF PROCESS MODELS

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Abstract

Mathematical process models can be applied in several different ways to serve industry by inducing beneficial changes to process operation. This paper attempts to summarize the different uses, types, and attributes of these models, and to offer some ideas to consider when developing, using, and reporting on 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 author's experience in modeling the continuous casting of steel.

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Introduction

The objective of this paper is to provide a partial introduction for this symposium by discussing some basic aspects of the application of mathematical process models in industry. Essentially, the aim is to explore how process models are used to benefit industry, and to offer some general comments and suggestions, based on the experience of the author, on how models can best meet this goal.

This work is concerned with process models, which consist of systems of mathematical equations and constants that are solved on a computer to make quantitative predictions about some aspect(s) of the process. The specific variables required as input data and generated as output data are important features of the model. The equations often derive 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, and usually require considerable effort to obtain. Thus, general-purpose commercial software packages, (ie. finite-element or finite-difference based codes), are not models in this context. They are useful tools, however, serving as frameworks for the development of process models.

As in any other endeavor, success in modeling is more likely when there are clear objectives. When developing, applying and reporting on the results from a model, a multitude of decisions must be made. In making these decisions, it is important to consider how and by whom the model will be implemented and to ask the question what good can it do.

Insights into the many ways to do effective process modeling can be found in previous work by prominent members of the modeling community [1-6]. This paper was inspired by the penetrating comments made by Joe Herbertson to the modeling community at the Modeling of Casting and Welding conference [1]. As a response from someone in the academic community, the examples in this paper are taken from the same process: the continuous casting of steel which is pictured in Figure 1.

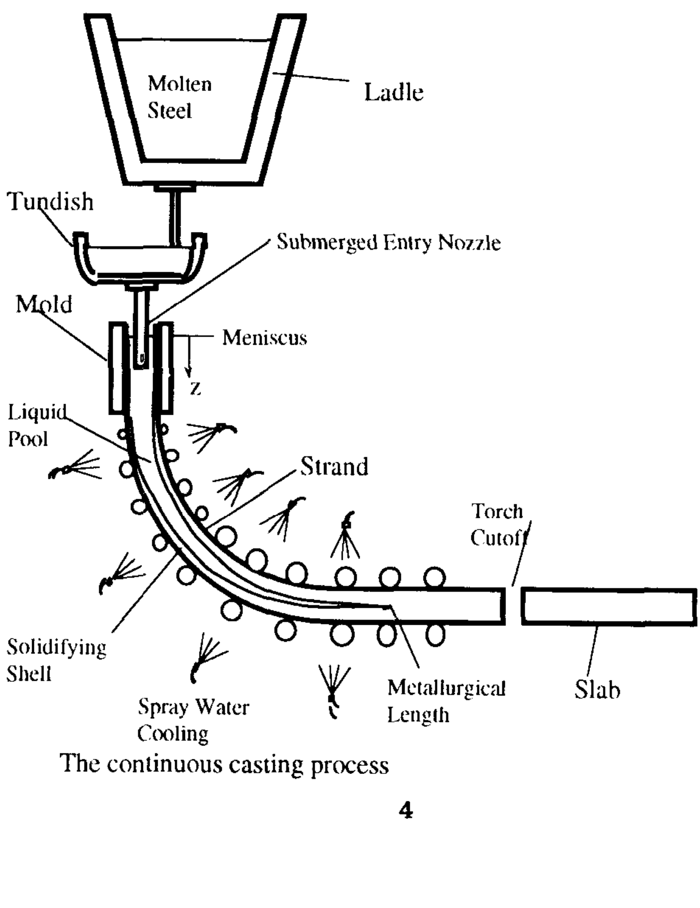

Figure 1. The continuous casting process

Hopefully, a better understanding of how models are implemented in practice will lead to more effective model implementation and avoid the all-too-common tragedy of models that are never implemented.

Definition of model implementation.

First, it must be recognized that the principal aim of industry is to make money. In materials-processing based industries, two possible ways to 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 a given defect by indicating achievable changes in the process. Note in the above comment the two key terms: "eliminate" the defect and "achievable" changes.

The ultimate goal of many process modeling efforts is to predict the occurrence of some kind of defect, such as segregation or cracks. 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 modeler, 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. The modeler 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. 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.

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

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 paper aims to explore how process models are implemented according to this definition, and to comment on the implications for process modelers.

Ways to implement a model

There are many paths to model implementation. In this work, process models are classified into types according to how and by whom the model results are implemented into practical process changes:

- fully-online models
- semi-online models
- offline models
- literature models

In practice, a continuum exists between these four idealized model types. The next sections define and examine how each type is implemented, in order of its immediate impact in industry.

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 [7] or moving temperature inversions, [8] 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 [7, 8].

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, or laboratory-scale measurements, or even sophisticated numerical experiments. 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 suggested by Brimacombe [9], have tremendous potential benefit to industry, as fully-online models of the future.

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 cost of model implementation and features required of the model. These models are best suited to indicating optimum levels to set for SOP variables, in order to account for gradual or infrequent changes in processing conditions.

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. 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, [9] 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 complicated 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. Another disadvantage is the need for costly operator intervention and supervision to implement the model results. 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.

Offline models

Offline 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 must then be 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 offline 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 offline model must have a thorough understanding of the process, in addition to understanding the model. The offline model is just one of the tools that can be used to help generate that process understanding. Model results are implemented in combination with the user's personal knowledge, obtained from plant, pilot-plant, and laboratory experiments, physical models, literature, and other sources.

Offline 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. Offline 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. Offline 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 offline model can play an important role in this regard. For example, the model of intermixing during a grade change discussed previously could be used offline 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.

General-purpose, commercial software packages, such as the finite-element codes FIDAP [10] and ABAQUS [11] have a role in this model category by providing a flexible "modeling framework", wherein a modeler can develop his own process model, possibly saving effort in model development. Alternatively, special-purpose software can be developed for particular aspects of a specific process of interest, (for example: CON1D [12] for heat transfer in the mold, and MIX1D [13] for intermixing during a grade change for the process of continuous casting of steel slabs). Models can also be developed for a specific aspect of a group of processes, such as a transient 1-D inverse heat conduction model that outputs the heat flux history needed to produce any arbitrary measured temperature profile, so long as the 1-D approximation is valid.

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. If a process model is too difficult to use, it may be easier to obtain the needed knowledge another way, such as through physical models, experiments, or even trial and error in the plant.

It is critical that the model have numerical integrity for all of its conceivable uses. The more the model is validated or calibrated with experiments, the better. It is also advisable that the person running the model have both a thorough knowledge of how the model works. The model developer should make it clear what the assumptions of the model are.

To help implement changes, offline models must be able to simulate process situations outside the scope of prior experience. Thus, the model should be as mechanistic and flexible as possible. 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 or calibration with experiments easier. Unfortunately, it also tends to complicate and slow down the model.

Online implementation of this type of model is limited primarily because the model is too slow, too difficult to run and too difficult to interpret by plant operators. The same flexibility that enables offline advances, can make the model difficult to use online. Sometimes, a simplified version of the offline model can be developed for online use.

Literature models

Literature models are defined here as offline models which are used only by the person(s) who developed the model. Furthermore, the modeler 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. Several indirect methods of implementation are discussed in the next sections. These models represent the majority of all models.

At their best, literature models can act as offline 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 offline 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 potential reader. 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 modeler 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 modeler to run.

Process models are very good at performing controlled parametric studies, particularly relative to plant-scale experiments, which are hard to control. The effect of each variable of interest can be systematically changed, in order to isolate the individual effects.

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 modeler make reasonable assumptions regarding both the phenomena included in the model, and the input conditions adopted in parametric studies. To do this, the modeler must obtain a sufficient understanding of the process to make reasonable choices and interpretations.

Before developing a process model, it is essential to have a qualitative understanding of the basic phenomena which govern the process. [5] This is because models, at best, can only quantify that understanding and shed insight into the interactions between the phenomena. The model cannot identify phenomena which have been neglected. Also, phenomena which are not understood mechanistically are not good candidates for process models unless comprehensive experimental data can be found.

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 Joe Herbertson [1] in Figure 2. 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.

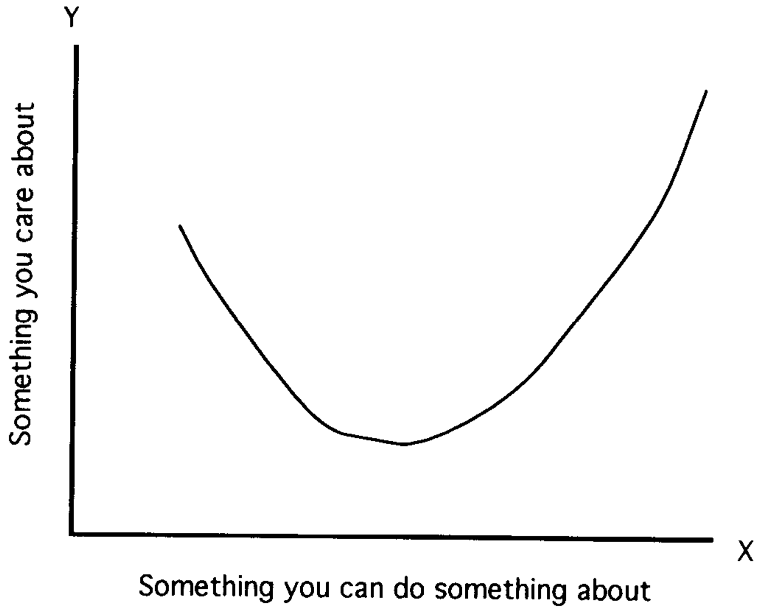

Figure 2. Graph containing results which can be implemented

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 modeler to continually strive for accurate modeling conclusions, by understanding the process of interest and validating the model.

Empirical versus mechanistic modeling

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.

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 fully-mechanistic process model could be extended to understand and solve any problem 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, although some literature models mislead by implying they are. In reality, it is possible at best to model mechanistically only a tiny fraction of the actual phenomena present in a real process. This 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
- 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
- thermodynamic reactions within and between the powder and steel phases
- 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 be! - the model would be too complex to ever run.