Metallurgical Process Modelling

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ABSTRACT: Computer Aided Process Modelling (CAPM) is applied in steelmaking in different areas from fundamental R&D to Online Process Control and for different application fields. An up-to-date introduction to the field is given by a general process model definition as well as a brief discussion of model properties and modelling concepts. In the framework of the current state-of-the-art and the underlying principles from fundamental physics to complex systems theory, process modelling is introduced as a tool to master increasing process complexity.

Illustrative examples enlighten the general advantages of the specific approaches and the specific drawbacks in the real world production environment. These examples are taken from own experiences with an EAF zone model and from the data available in the open literature.

The vision of Metallurgical Process System Engineering with Model Predictive Control of metallurgical processes by detailed Computational Fluid Dynamics based Process Models is obvious.

1. INTRODUCTION

A decade after the well known review on process modelling from a metallurgist point of view by Thomas and Brimacombe [1], this paper makes an attempt to update and discuss the general issues on metallurgical process modelling. Special emphasis will be taken to provide a widely acceptable definition of the term “process model” and the requirement of clear software interfaces between the process models and industrial control and optimization systems.

This paper is an attempt to stimulate cooperation by providing a common understanding for model developers and end users. The term process model is used for a specific class of models used in process metallurgy as defined below. The following classes of “models” are not included: databases, neural networks, general data analysers (stochastic or deterministic) and all other “models” not based on fundamental conservation principles and scientific process analysis. This is not a valuation of models based on automated experimental data compression and not requiring additional scientific process knowledge – they may deliver sufficient results as long as

- no significant extrapolation capability is required (e.g. for process optimization or new process development).
- a significant amount of experimental process data is available in advance.
- no data on immeasurable quantities (e.g. the remaining solid material during meltdown in an EAF) is required.

These non mechanistic models are often not very interesting for most metallurgists – they do not provide or enhance process understanding. For practical reasons, the common software interfaces can be defined and used for most classes of models.

2. THE TASKS OF A PROCESS MODEL AND ITS OUTLINE

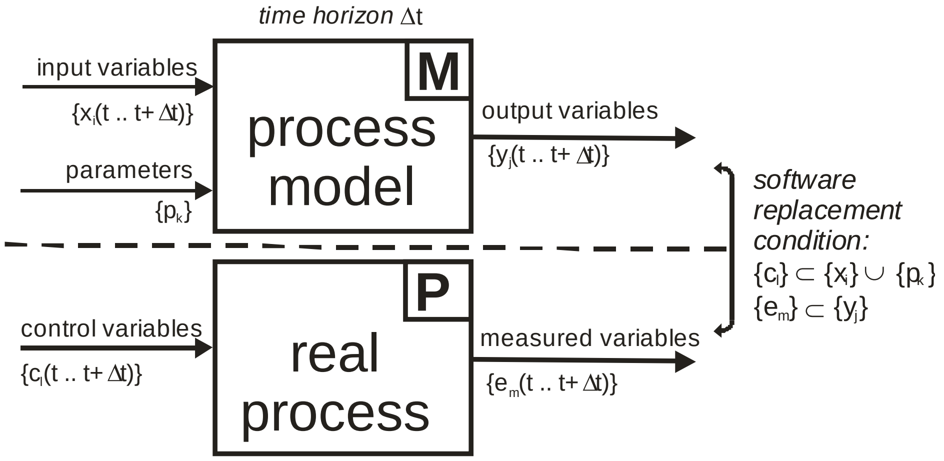

Fig. 1: Process model as a software replacement of the real process

Similar to the "system of mathematical equations" definition [1], a process model is defined as an implementation of an *algorithm to predict the behaviour of an open or closed system* as sketched in Fig. 1. The information on the current system state is stored in the models internal memory and as long as the software replacement condition is fulfilled, the model can be used to simulate the reality. Such a process simulation is a subset of process modelling as it is an experiment performed on a model. As a conclusion, a process model supports concept, design and operation by delivering the software implementation of the real process. To some extend expensive or dangerous experiments can be replaced by process simulations.

For the industrial users, metallurgical process models should allow to perform all modelling tasks during the process lifecycle, providing some of the following benefits:

- Online determination (automation level 2) of quantities which can not be measured (e.g. the amount of solid during meltdown in an EAF) or where continuous measurements are not available (e.g. melt mass and temperature control).
- Operator assistance and model based predictive process control (level 2).
- Shop automation (level 3) support by data analysis for automated optimisation of control parameters and production planning.
- Parameter estimation and computerized design experiments for process optimisations, novel processes and formal risk analysis.
- Offline process optimization with a minimum number of experiments (level 2.5).

For the process researchers and developers, process models can provide some additional benefits:

- Analysis of real plant data by inverse modelling for the determination of process parameters (e.g. heat-, mass- or species transfer coefficients) which can not be determined by independent experiments.
- Real world tests for the predictive power of mathematical modelling.
- Enhanced understanding of the underlying physical mechanisms by the comparison of experimental correlations with calculated parameter sensitivities (hypothesis testing).

3. THE DEVELOPMENT OF PROCESS MODELS

The end-users of process models are mostly shop operators and junior engineers. They require specific user interfaces procured by automation system experts or other IT personnel. Those IT-experts require well documented and simple interfaces (see below). For process model developers in metallurgical industry as well as their suppliers, the question of know-how acquisition and protection is as important as long term reliability. For big and complex metallurgical reactors (BF, EAF, BOF, ..) proprietary process models are state of the art. Because these models are often plant specific, some standardisation and interfacing is required for the comparison of competing models. Such open interfaces can make proprietary models compatible with general purpose process modelling systems [2, 3]. These systems can be helpful in standardized automation environments as long as their complexity is not consuming too many resources.

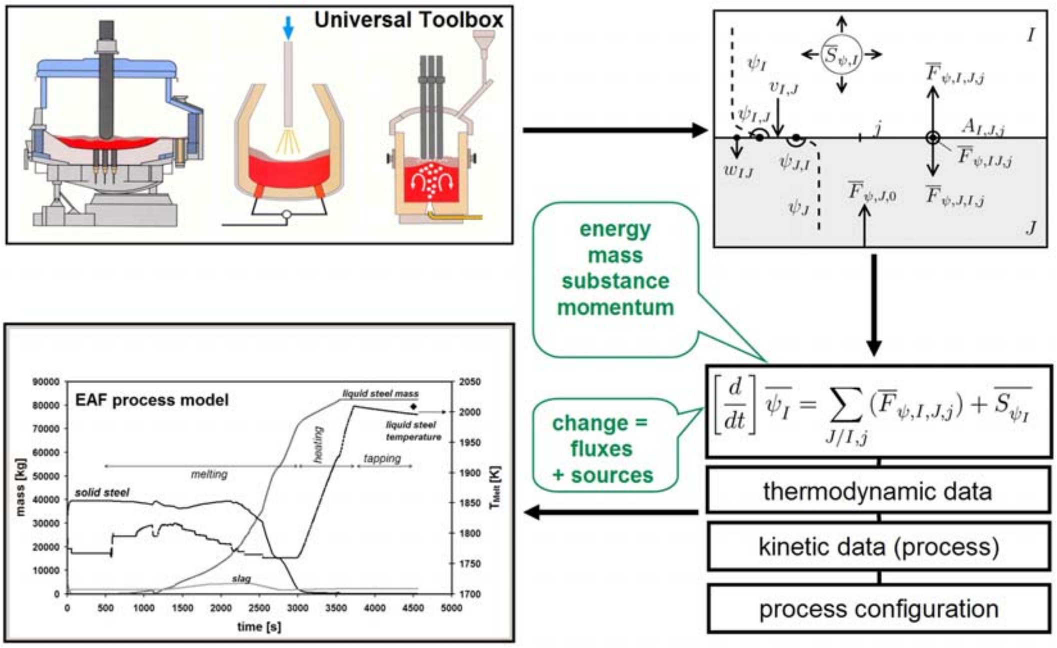

Fig. 2: Zone based process modelling.

The most efficient way to develop a process model is to make a specific model with general purpose interfaces. As sketched in Fig. 1, a process model of a specific metallurgical process is developed by dividing the device into a small number of zones. For each zone, energy, mass, species and momentum is balanced. This may be a global or a detailed (e.g. using CFD solvers) model for the individual zone. The time dependent change for all individual zones (which may come from a toolbox of predefined sub-models) is determined from the ODE system for each quantity to be balanced. Finally the process model predicts the process quantities as detailed as possible for the given zone partitioning. Such models where developed for a number of metallurgical processes, e.g. the EAF [4,5,6] or the RH refining process [7]. For an introduction into the mathematical modelling of metallurgical processes refer to the textbooks [8,9,10]. In practice, the real world complexity links process model development with the process lifecycle itself (Fig. 3).

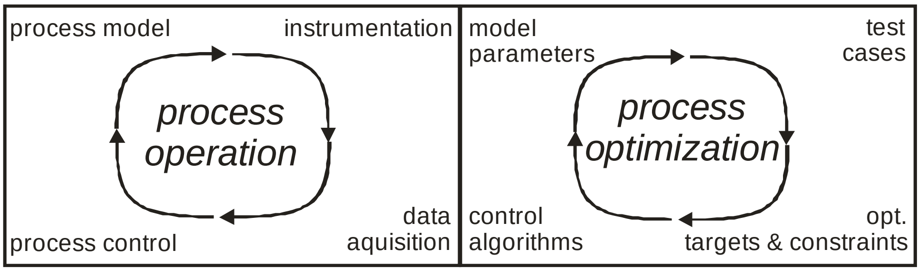

Fig. 3: Process (model) development cycle.

3.1 The user/developer interface

For maximum acceptance, rapid development and high quality modelling, there must be a clear and easy to understand software interface to the process models. Such an interface has two major parts – both should be as transparent as possible:

- A general purpose calling convention suitable for all process models and useable from all major programming environments and general purpose modelling systems [11].
- A process specific Input(x_i, p_k) / Output(y_j) data definition with long term downward compatibility and simple interfaces for newcomers [11].

Both have to be as simple as possible – but not simpler. For the model calling convention, a general, i.e. process un-specific, interface is proposed [11]. The process specific definition of the input data x_i, the process parameters p_k and the output data y_j must be a compromise between flexibility, compatibility and the automation system requirement to minimize the total number of values to be exchanged between the process model and the level-2 system. A strategy of starting as simple as possible and add more complex but compatible new versions is proposed [11]. The different levels of end-user experience require strong default value setting and range checking inside the model.

This interface is compatible to other programming languages like FORTRAN (using null character padding for strings) and it provides full flexibility as well as the possibility to sustain compatibility between different process models [11]. The interface is accompanied by detailed specifications (x_i, p_k, y_j) for individual models predicting specific processes [11].

4. THE INFRASTRUCTURE, ENVIRONMENT AND IMPLEMENATION OF PROCESS MODELS

The information technology (IT) environments for process models have seen some type of consolidation during the last decade. Offline operation is mainly done on standard PC workstations under Windows and Linux operating systems. Actually, online operation may require the integration into proprietary hardware provided by the automation system vendor since long term spare part delivery is required. In the future, hardware virtualization technology permits the long term operation of process models running inside dedicated virtual machines. Since single CPU computer performance is limited, parallelization may become important in the future. Main memory and hard disk space is no longer a limitation while data transport is more often limiting the model performance. While earlier process models were often implemented as monolithic FORTRAN codes, programming environments nowadays support mixed language programming. For maximum performance C[++] and FORTRAN programming is still recommended while object oriented computer languages like Java and C++ are most cost effective as long as qualified programmers are available. As a rule of thumb, the infrastructure and implementation language must be adapted to the process experts in the developer team while for the end users only the interface needs to be documented (see 3.1).

5. EXPERIMENTAL VALIDATION, SENSITIVITY ANALYSIS AND QUALITY ASSURANCE

5.1 Experimental validation and parameter determination

For a given set of model parameters, the model can be used to predict measureable values for a number of real world experimental data sets. By a quantitative comparison of the predicted with the measured values, the process model can be validated. Most models are not ab initio, i.e. they contain process specific parameters. These parameters can be obtained by independent measurements and/or inverse modelling procedures: The parameters are varied until the mean deviation between the measured and the predicted output values (e.g. melt temperature) reach a minimum. As a consequence, validation and parameter determination requires differing data sets.

5.2 Sensitivity analysis

All process models have measured input parameters with limited accuracy (e.g. weighting errors) and model parameters with limited or even unknown correctness. The so called sensitivity analysis is an effective mean to determine the critical model parameters and the accuracy of the output data with respect to the accuracy of the input data [12].

As an example, the prediction of the EAF tapping temperature by ±10 K (0.5%) requires an accuracy of the weighting systems (scrap, DRI, ...) of 0.5%, and 0.4% for the input power measurement while the heat transfer coefficient between solid and liquid can have an uncertainty of 8% [4]. With the help of an initial process model, the sensitivity analysis can provide information on the principal accuracy of the predicted output data as a function of the input and parameter data accuracy (sensitivity map).

5.3 Quality assurance

The quality of process models can be categorised into the fields software stability, maintainability, prediction capability and compatibility. The quantification of quality is not a trivial task and is strongly connected to the complexity management in order to avoid too much “unknown unknowns” in the process itself and “unknown knowns” in the model.

5.3.1 Prediction capability

The prediction capability of a process model can be determined after the model parameters and the sensitivity map are known. For a specific direction (e.g. time, i.e. the prediction of the process future), the prediction capability of the model will be the difference between the predicted and the measured values compared to their absolute variation and the time horizon. In the prediction capability calculation, differences are counted only if the model can be responsible for the deviation. E.g., if process additions weighting error results in a 10 K melt temperature uncertainty, only deviations above 10K can be counted.

5.3.2 Model comparison and benchmarking

Actually, the author found no quantitative comparisons of process models in the open literature. As soon as general purpose user/developer programming interfaces will be accepted [11], benchmarking and detailed model comparison will be possible. This will be a major step towards model validation and benchmarking.

5.3.3 Common model limitations and pitfalls

Often models are thought to be limited by their underlying databases and scientific simplifications and assumptions. Since regular scientific efforts can deal with these limitations, they are often present but seldom critical. Critical limitations can come from unknown scientific information (e.g. reaction rates) which is unaffordable to measure and difficult to obtain by inverse modelling. A common pitfall lies in the datasets used for validation. As an example, an EAF process model test using data for a single furnace operated always in the same manner may deliver apparent excellent results even for a poor model. In order to avoid a false positive parameter fitting procedure, different operating regimes must be described by the same parameter set.

As a conclusion, the general rules of science must be strictly kept (no Procrustes- or Pygmalion-like behaviour). Most process models have a large number of fittable parameters. They should be specified and traced back to fundamental science rather than being adapted to specific data sets and finally generating false positive model validations.

6. CONCLUSIONS AND FUTURE CHALLENGES FOR PROCESS MODELLING

While the “devil is in the detail” also for metallurgical process models their development and application can benefit from a general purpose software interface and compatible Input/Output specifications for the individual processes. There seems to be a general agreement on the underlying fundamental science and the usage of thermodynamic databases.

The major challenge in process modelling will remain in the field of complexity management. The often propagated *general purpose* process models have difficulties to fulfil the requirements for processes unaccounted during their development. Additionally, current and future metallurgical processes will remain complex and will be part of complex production systems. Instead of general purpose process models the model developers will use construction kits with more and more integration of external scientific computing software.The IT development may allow to address the following issues in the future:

- Integration of engineering simulation solutions as well as open source packages for the large scale parallelized solution of multi-physics PDE systems on unstructured grids into process models even for online applications.
- Model Predictive Control (MPC) [13] using non-linear process models will be applied to metallurgical automation systems.
- Simple common interfaces [11] will speed up the integration of process models into standardized automation (HMI/SCADA) systems and will allow independent off-site model development.
- The Online/Offline model distinction may vanish due to increased performance.
- Process specific databases will be replaced by general purpose thermodynamic databases and thermo chemical software packages.
- Benchmark problems and data sets will allow for a quantitative comparison of different models for the same process – increasing transparency and quality of the individual models and increasing the acceptance of process models even for mission critical applications like model predictive control (MPC).
- Computer Aided Process Engineering (CAPE) can support process development in metallurgical industry.

Model quality will become an industrial issue because the model end-users may force their system suppliers to deliver solutions with open interfaces suitable for independent quality control. The vision of Process System Engineering with Model Predictive Control of metallurgical processes using detailed Computational Fluid Dynamics based Process Models is obvious. More and more advanced simulations of transport phenomena will be integrated into process models increasing their predictive power but also their complexity. Common software interfaces will allow the rapid model transfer from laboratory to plant automation systems.

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