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Cross-sectorial real-time sensing, advanced control and optimisation of batch processes saving energy and raw materials (RECOBA)

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Final model layout as a guide/tutorial for interested parties outside of RECOBA consortium

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1 Introduction

Although the industrial (semi-)batch processes that are subject of real-time optimization in the RECOBA project share several common characteristics, e.g. temporal evolution of product/intermediate product quality or importance of temperature control, they also significantly differ in their fundamental aspects, e.g. number of interacting phenomena, number of chemical components involved or influence of macro-scale dynamics. These differences were reflected in the mathematical models, which were developed within Work Package 4 for on-line control and optimization applications.

In Deliverable D 4.1, the layout of the process models which were available for (i) polymerization, (ii) steelmaking, and (iii) silicon production processes at the beginning of the project, and which were subject of extensions developed throughout the work performed within WP 4, has been described. This layout is now updated and generalised in this Deliverable D 4.7, to provide cross-sectorial concepts and strategies for development of dynamic process models, which are detailed enough for accurate process description, but nevertheless sufficiently fast for application within on-line control systems. The final model layout thus shall serve as a guide/tutorial to interested parties (outside of RECOBA project consortium) how to quickly interface their batch process models with optimisation and control tools.

2 Structure and interfaces of process models

In this section first a description of the structure and functionality of the process models which were developed for the different (semi-)batch processes involved in the RECOBA project is given, with focus on (i) model inputs available from real-time process sensing (online process measurements), (ii) predictions of the relevant process state variables and product characteristics and (iii) modular architecture, i.e., interconnection of separate model parts constituting the desired control model.

Next, the interfaces of the models for integration within on-line control and optimisation tools are outlined.

Both aspects are generalised for application of the approaches at other batch processes of the process industry.

2.1 Model structure and functionality

2.1.1 Polymerization process

The polymerisation process considers a seeded emulsion polymerisation, during which a second polymer phase grows within already existing polymer nanoparticles, so the models have to take into account different scales. Spatial scales span from macro-scale properties relevant for the whole reactor to nanoscale properties relevant to polymer nanoparticles present in the polymer dispersion and even molecular architecture of polymers within the polymer particles. For this purpose, we use different models to describe properly all physical and chemical processes in the system. Namely, three models are used: Macroscale deterministic model capturing monomer(s) conversion and temperature development within the reactor; Morphological deterministic model describing evolution of the two polymer phases present in the polymer particles and consequently influencing particle morphology; and stochastic Monte Carlo model simulating growth of the polymer molecules in the particles and thus predicting polymer properties. Here we describe individual models' functionalities and finally their common interconnections.

2.1.1.1 Macroscale model

This model is based on a set of ordinary differential equations (ODEs), which describes evolution of all different species present in the reactor (monomers, polymers, chain transfer agent – CTA, water, initiator, surfactant and water) in all phases (aqueous phase, oil phase and polymer particles), transport phenomena of the species between the phases and chemical reactions of all species. An input for this model is a recipe, which describes the initial conditions in the reactor and feeding profiles of individual species in time (monomer, initiator, CTA, surfactant and water). Output of this model is the time-evolution of all species concentrations and consequently mainly monomer(s) conversion and temperature evolution. List of all state variables balanced in the model is collected in Table 1.

Table 1: List of state variables of the polymerization process mode

Name	Symbol	Unit
Molar amount of monomer M1 in the system (particles + droplets)	n_{M1}	mol
Molar amount of monomer M2 in the system (particles + droplets)	n_{M2}	mol
Molar amount of monomer M3 in the aqueous phase	n_{M3}	mol
Molar amount of monomer M4 in the aqueous phase	n_{M4}	mol
Molar amount of water in the aqueous phase	n_W	mol
Molar amount of CTA in the system (particles + droplets)	n_{CTA}	mol
Molar amount of undissociated initiator in the aqueous phase	n_I	mol
Molar amount of redox inhibitor in the aqueous phase (in case of redox initiator usage)	n_{redox}	mol
Molar amount of monomer M1 in polymer particles	n_{M1}^P	mol
Molar amount of monomer M2 in polymer particles	n_{M2}^P	mol
Molar amount of CTA in polymer particles	n_{CTA}^P	mol
Molar amount of polymerized M1	P_{M1}	mol
Molar amount of polymerized M2	P_{M2}	mol
Molar amount of polymerized M3	P_{M3}	mol
Molar amount of polymerized M4	P_{M4}	mol
Average number of radicals per polymer particle	\bar{n}	-
Molar amount of radicals in the aqueous phase	n_R^W	mol
First moment of living chains	μ_1	mol
Zero moment of dead chains	λ_0	mol
First moment of dead chains	λ_1	mol
Temperature of reaction mixture	T_R	K
Temperature of the reactor jacket	T_J	K

2.1.1.2 Morphological model

Inputs of the Morphological model are conversions of individual monomers (gained from the Macroscale model) and balances generation, growth and position of the second polymer clusters in the particles. The clusters are divided into two groups according to their position to non-equilibrium (typically inside the particles – at the place of their birth) and equilibrium (typically the edge of the particles). Furthermore, these two groups of clusters are divided into a distributions according to their size (volume of incorporated polymer), which corresponds to the fact that a set of particles gives us distribution of different morphologies influenced by the distribution of the clusters (*cf.* Figure 1 left). The clusters distributions are divided among a finite number of pivots, which gives us a finite number of variables to be balanced. The resulting model can predict an evolution of clusters distribution, which example is depicted in the right of Figure 1.

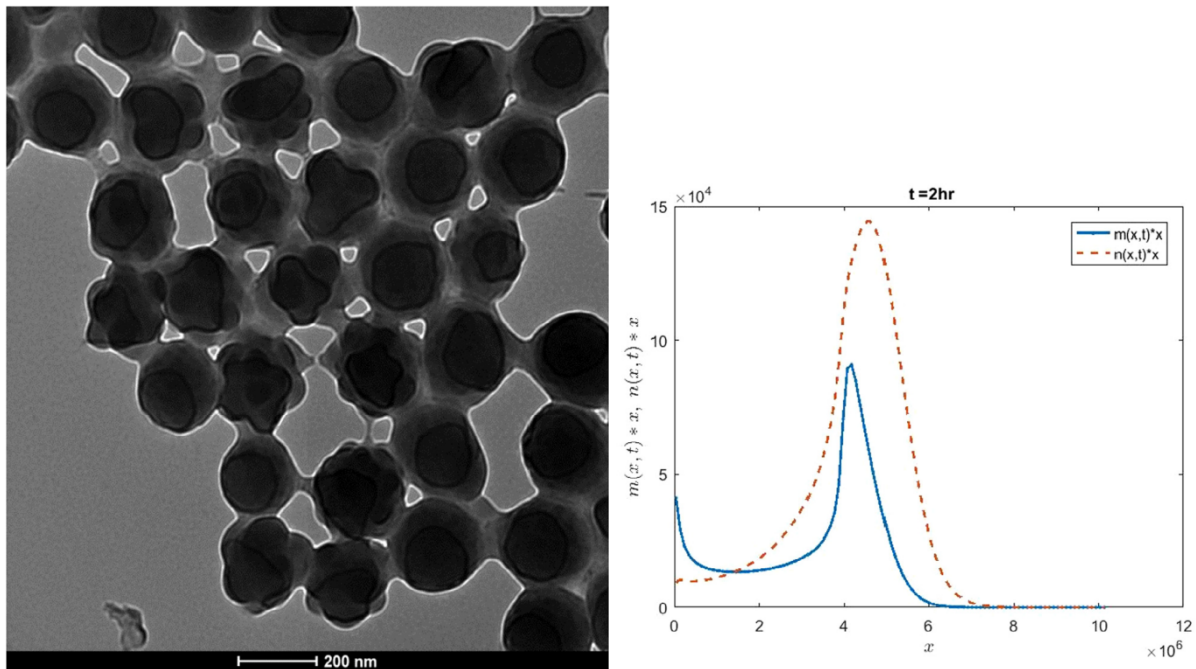


Figure 1: Left figure is a TEM micrograph of composite latex produced by seeded emulsion copolymerization of styrene and butyl acrylate on a methyl methacrylate-butyl acrylate crosslinked seed illustrating distribution of particle morphologies [1]. Right figure depicts normalized weight distribution of the equilibrium, $n(x,t)$, and non-equilibrium clusters, $m(x,t)$, present in the system predicted by the Morphological model [1].

Morphological model is also encoded as a set of ODEs and therefore it can be easily implemented as an extension module of the Macroscale model. The equations can be integrated either simultaneously with the Macroscale model or as a second step using precomputed concentrations. Integrating in two steps is better for numerical stability (because the two systems have different stiffness) and for control purposes, because the computational demands are different (morphological model, although quite fast, is still several times slower).

The innovative morphological model can describe any multiphase system in which the morphology of the phases is driven by reaction generation of one phase and its diffusive migration towards an equilibrium position. Model structure would be similar for all such systems; however, constants describing individual phenomena in the system (e.g. nucleation, migration, coalescence of the clusters) might have different physical meaning and consequently different values or even different functional dependencies.

2.1.1.3 Monte Carlo model

Most of the polymerisation takes place in the separated polymer particles and number of radicals (reaction centres) in each particle is typically on the order of ones, which is not reasonable to be treated as a continuous variable. There are approaches, how to properly approximate these rather discrete than continuous

variables for differential purposes, but stochastic approaches are more natural for such systems and, therefore, sometimes more efficient. To make the model more computationally efficient we used a hybrid approach, which uses precomputed concentration profiles from the Macroscale deterministic model and focuses only on simulating of polymer chains and their interconnection (branching) in the particles. This approach reduces computational time of hybrid Monte Carlo method below 10 seconds even for the copolymerisation of 4 monomers, so that requirements for online process control are met.

The model is implemented as an extension module to the Macroscale model. Monte Carlo needs as an input results from Macroscale model and further provides predictions of full molecular weight distribution and molecular architecture.

References

[1] S. Hamzehlou, J. R. Leiza, J. M. Asua, A new approach for mathematical modelling of the dynamic development of particle morphology, *Chem. Eng. J.* 304, 2016, 655-666

2.1.2 Steelmaking process

For the different batch processes of the liquid steelmaking process, the focus was laid on modelling of the evolution of the melt temperature. For this purpose, also the thermal state of the refractory lined reactors (steel ladle and vessel for vacuum treatment) had to be acquired in a detailed manner. Additionally the thermal effect of the various metallurgical reactions which are performed within the different aggregates of the process route, such as decarburisation and deoxidation, had to be taken into account within the model calculations. Also the effect of material additions (alloy and deoxidation materials, slag formers etc.) on the melt temperature had to be considered.

Regarding modelling of the melt temperature evolution, the complete chain of batch processes from tapping of the steel melt into the ladle at the converter up to the delivery of the melt to the continuous casting plant was taken into account. Fig. 2 shows this part of the process route of liquid steelmaking in more detail.

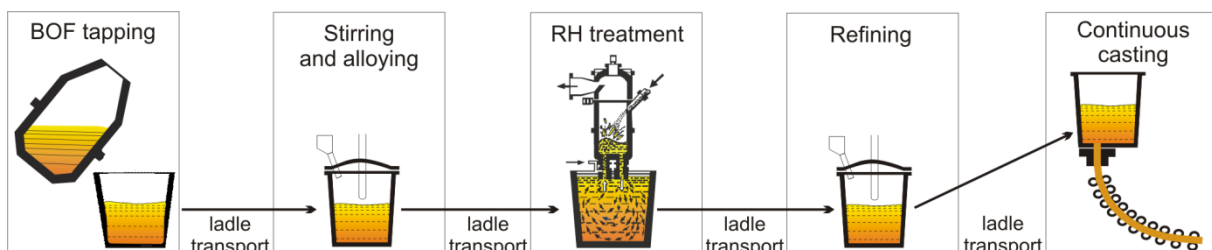


Figure 2: Chain of batch processes for ladle treatment of the liquid steel melt.

In accordance with the requirements of the steel plant at TKSE, a detailed modelling of the liquid melt temperature evolution was performed for the RH vacuum degassing plant and the gas stirred ladle treatment station for final refining of the steel melt. In these aggregates the final adjustment of the liquid melt temperature is performed according to the requirements of the continuous casting plant. Also the continuous in-line measurement of the melt temperature has been applied and tested at these aggregates.

The dynamic process models can be used for on-line monitoring and prediction of the evolution of the process state with focus on the melt temperature for the entire chain of batch processes for liquid steelmaking. In this sense the models can act as soft sensors to provide information on the evolution of the process state variables, especially of the melt temperature, which are so far not measurable in a continuous manner.

The process models are based on dynamic energy and mass balance calculations, in combination with thermodynamics and reaction kinetics of metallurgical reactions with significant energy input due to their reaction energy (e.g. decarburisation and deoxidation reactions). The result of the energy balance calculation can be adapted to each reasonable spot temperature measurement performed with a thermocouple probe.

The model calculations are implemented as non-linear differential and algebraic equations with stepwise defined model parameters for the different batch processes of the process chain.

The real-time applicable process models also consider the effect of the thermal state of the refractory-lined metallurgical reactors on the melt temperature. For that purpose the refractory temperatures of ladle and vacuum vessel were included as separate state variables. From the temperature difference between inner wall of the vessels and melt temperature, the related melt temperature loss rates were derived.

Input data for the process models are:

- initial heat state, i.e. temperature, weight and composition (especially regarding C, O, Al, Si) of the steel bath at the beginning of ladle treatment, i.e. when the melt is tapped from the oxygen steelmaking converter into the ladle
- initial ladle and vessel state, derived from characteristic data of ladle and vacuum vessel history influencing their thermal state (e.g. ladle and vessel empty times, ladle and vessel filled times during previous treatment etc.)
- cyclic process data, i.e. mainly lance stirring gas flow rates, RH lift gas flow rate, lance oxygen flow rate and vessel pressure of vacuum treatment,

- acyclic event data, i.e. mainly material additions (alloy and deoxidation materials, cooling scrap, slag formers), samplings of steel with laboratory analyses, temperature and oxygen content measurements.

These input data are required on the one hand to feed the dynamic model calculations, and on the other hand, with regard to the spot measurements of the heat state variables (steel bath temperature and analysis) to allow their validation.

The following heat state variables are calculated continuously over time as outputs of the model:

- current melt temperature
- current temperatures of refractory wall of the ladle and the vacuum vessel
- weight and composition of steel bath (especially regarding C, O, Al, Si)

along the complete chain of batch processes for ladle treatment at the different aggregates from tapping to final stirring. A list of the most important state variables is given in Table 2.

Table 2. List of state variables for the steelmaking process models.

Name	Symbol	Unit
Steel bath temperature	T_B	K
Inner wall temperature ladle	T_{WL}	K
Inner wall temperature RH vessel	T_{WRH}	K
Carbon content in steel melt	c_C	wt%
Oxygen content in steel melt	c_O	wt%
Aluminium content in steel melt	c_{Al}	wt%
Silicon content in steel melt	c_{Si}	wt%
Mass of steel melt	m_m	kg

The process models were implemented as MatLab / Simulink application for offline simulation, to validate the model calculations by comparison to spot measurements for selected state variables as steel melt temperature and composition. Within this validation procedure, also the model parameters were identified which lead to an optimal model accuracy with respect to the melt temperature.

Within an on-line process monitoring application, the dynamic process models can provide the actual process state variables within a cycle time of less than 10 seconds. This is appropriate with respect to the dynamics and kinetics of the involved processes. For application within real-time control tools as MPC, the models can provide prediction results regarding the melt temperature evolution within less than 1 s, which allows also iterative optimization calculations.

2.1.3 Silicon Production Process

The ladle refining process for silicon production was described in detail in RECOBA Deliverable D 2.3. The offline model RafSim models the refining by following the flow of gas bubbles from the bottom of the ladle, where they are injected through a bottom plug, up to the bath surface. The gas is a combination of air and oxygen. The model calculates the concentrations of the different elements present on the slag film surrounding the bubble as it rises to the surface. When a set of bubbles reaches the surface, the model updates the bulk concentrations with the contributions from both the bubbles and surface reactions.

The model can be seen as quasi-dynamic, describing both time and position variations by ordinary differential equations. The time variations describe the ladle dynamics, while the position variations are related to the vertical position of a gas bubble at a given time stamp.

The reactions included in the model describe the formation of SiO₂-CaO-Al₂O₃ slag from adding a mixture of air and oxygen to the metallic melt. The model divides the slag into one homogeneous and one inhomogeneous part. The current model formulation results in 12 state variables listed in Table 3 below.

Table 3: State variables for offline silicon refining model.

Name	Symbol	Unit
Aluminium level in melt	c_{Al}	wt%
Calcium level in melt	c_{Ca}	wt%
Number of mol SiO ₂ in inhomogeneous part of slag	$n_{SiO_2}^i$	mol
Number of mol Al ₂ O ₃ in inhomogeneous part of slag	$n_{Al_2O_3}^i$	mol
Number of mol CaO in inhomogeneous part of slag	n_{CaO}^i	mol
Number of mol SiO ₂ in homogeneous part of slag	$n_{SiO_2}^h$	mol
Number of mol Al ₂ O ₃ in homogeneous part of slag	$n_{Al_2O_3}^h$	mol
Number of mol CaO in homogeneous part of slag	n_{CaO}^h	mol
Temperature in melt	T_m	K
Temperature in ladle refractory	T_w	K
Scull thickness	d_{skoll}	m
Mass of melt	m_m	kg

The variables are updated for each time step.

The model divides the surface slag into one homogeneous and one inhomogeneous part. The extent of contact between the two parts is described by the area ratio of the inhomogeneous and homogenous part, which is again related to the volume ratio of the two parts multiplied by a user-defined parameter.

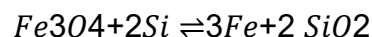
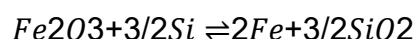
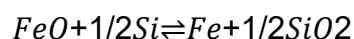
The additives are at first added to the inhomogeneous part, and then transferred to the homogenous part during a time period defined by the user. If the time period in between two successive additives of the same material is shorter than the user-defined period, then the first additive will be transferred to the homogenous part during the period in between the two additives.

It is assumed that all slag is contained in the homogenous part at start-up. For each time step, the concentration of Al (Ca)(Mg) in the melt is updated:

- Reaction with top slag, given by the distance from equilibrium of slag to melt together with the corresponding mass transfer coefficient. This is a separate calculation for the inhomogeneous and homogenous part of the slag
- Reaction on the bubbles given by the amount of slag film created for each time sample
- Difference in concentrations of Al (Ca)(Mg) in the ladle melt and the furnace tapping stream. The tapping feed rate and the composition of the feed from the furnace are collected from user-defined tables for each sample and can therefore be configured to be time variant
- Additions

The desire to avoid negative concentrations in the melt leads to upper limits for the terms. Also, to avoid negative amounts of oxide in the slag additional lower limits are set.

Fe is not refined to oxides, but oxides added to the melt will react with silicon in the melt and give iron, as shown below:



The iron concentration in the melt thus increases by

- The difference between concentration of Fe in the ladle and in the feed from the furnace. The iron content from the furnace and the feed rate \dot{m}_{feed} are found from a table each time step, and can therefore be configured to vary with time
- Indirect by addition of iron oxides
- Direct addition

During one time step the amount of SiO₂ in the homogeneous part of the top slag is changed by:

- Reaction with O₂ from the air above the ladle.
- The amount of oxygen that reacted in one set of bubbles less the oxygen that has formed Al₂O₃, CaO and MgO at the surface of the bubbles.
- SiO₂ transferred from the heterogeneous part of the top slag.
- The reaction with Al, Ca and Mg from the melt given by the chemical driving force due to incomplete equilibrium between slag and melt, with its respective mass transfer coefficient.

During one time step the amount of SiO₂ in the heterogeneous part of the top slag is changed by:

- The reaction with Al, Ca and Mg from the melt given by the chemical driving force due to incomplete equilibrium between slag and melt, with its respective mass transfer coefficient.
- Additions of SiO₂ and indirectly by additions of CaCO₃ and iron oxides.
- SiO₂ transferred to the homogeneous part of the top slag

The refining reactions for Al, Ca and Mg give changes to the homogeneous or heterogeneous part of the slag, depending on which slag part the reaction refers to. The transfer between heterogeneous and homogeneous slag happens with a given fraction of the remaining inhomogeneous slag each time step, given by a parameter chosen by the user, which tells how many time steps this transfer shall take.

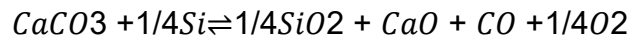
During one time step, the amount of Al₂O₃ (CaO)(MgO) in the homogeneous part of the top slag is changed by

- Reaction with the melt, given by the distance from equilibrium between slag and melt, together with the mass transfer coefficient.
- Slag added from one set of bubbles per unit time.
- Mass transfer from the heterogeneous part of the slag.

During one time step, the amount of Al₂O₃ (CaO)(MgO) in the heterogeneous part of the top slag is changed by

- Reaction with the melt, given by the distance from equilibrium between slag and melt, together with the mass transfer coefficient.
- Solid additions, for CaO also indirectly from CaCO₃
- Mass transfer to the homogeneous part of the slag

Indirect addition of CaO from CaCO₃ is described by CaCO₃ reacting with Si to SiO₂, CaO, CO and O₂ as shown below:



The metal in the ladle is cooled by (enthalpy losses)

- Heating and melting of solid additions of Si, Al, SiO₂, CaO and Al₂O₃
- Heating of the gas through the bottom plug, O₂ and N₂.
- Heat losses by conduction through the ladle walls and bottom.
- Heat losses by radiation from the surface of the melt.
- Endothermic reactions involving Al₂O₃, CaO, SiO₂, SiO₃, CaCO₃, FeO, Fe₂O₃ and Fe₃O₄

The metal in the ladle is heated by additions of hot metal from the furnace, as well as exothermic reactions such as the oxidation of Si.

The ladle wall temperature is found from the heat equation, where a temperature change is caused by a change in the conductive heat flow, and the temperature is fixed at the ladle exterior.

For a complete heat balance, the heat transfer between different regions of the ladle refractory should be considered, for example between side walls and the bottom region of the ladle. However, simulations showed that these contributions are negligible compared to the heat transfer directly through the walls, so a simpler, though somewhat less accurate, model was chosen. Generally, the heat transferred through the ladle lining is a small fraction of the total heat losses which mainly is caused by free surface radiation from the top.

The amount of melt in the ladle is for each time step changed by:

- Metal tapped from the furnace
- Addition of fines/cooling metal
- Skull formation
- Slag formation, where one mol reduction in SiO₂ from a refining reaction or reaction with additions gives one mol Si increase and vice versa. The increase in SiO₂ from addition of SiO₂ will not change the amount of Si directly, so this is not taken into account.
- Impurities that have left the melt
- Addition of Fe and Fe oxides, Al, Ca and Mg

Two remaining states, "skulls" and "old skulls" both have the same structure. They describe the skulls made during the current tapping and the ones remaining from earlier tappings. Each structure contains at least 2 elements, one element describing the skulls at the ladle bottom, and one or more elements describing the skulls along the ladle walls.

2.1.4 Generalisation of model structure for other batch processes

The description of the structure of the models for the different batch processes given above clearly reveals the similarities of the liquid steelmaking and the silicon refining process. Both are high temperature processes, which induces that a continuous and direct measurement of the relevant process state variables (mainly temperature and composition of the melt) is not possible. This emphasizes the need for a dynamic process model, which allows to describe the evolution of the process state variables in a continuous and real-time manner. This can be done by ordinary differential and algebraic equations. In combination with thermodynamic equilibrium calculations for the metallurgical reactions, these equations become non-linear.

In addition, for dynamic modelling of the high temperature processes to be used in real-time applications, it has to be assumed that the melt is homogeneous with respect to temperature and composition during the whole process time. A spatial resolution of the model calculation would increase the calculation time enormously, far beyond the 10 seconds which can be normally realised with such a dynamic model. At least for the steelmaking and the silicon refining processes this assumption is acceptable, as the melt is normally stirred well by argon gas injection.

Considering these preconditions and assumptions, the model structure which has been set up for the steelmaking and the silicon refining process can be transferred to other, similar high temperature batch processes.

For the polymerisation process, measurements at low temperatures (usually below 100 °C) are not such a problem, but all reactions within the process are highly temperature dependent. These reactions influence microstructure of the polymer particles (both molecular architecture and morphology), which is hardly measurable. The microstructure determines desirable macroscopic product properties. Therefore, models estimating these properties based on temperature development are extremely useful for online control.

The morphological model developed by PMAT predicts evolution of different phases during the polymerisation process. The model is encoded as a set of ODEs, so it is easily usable for online control of any multiphase system.

It was also shown that not all microscopic properties could be easily determined by continuous formulations of the model. In these cases, stochastic approaches are more suitable, but control algorithms require besides fast computing models also continuous predictions. Therefore, we presented a surrogate model, which is applicable for online control. These surrogate models are applicable in any system which requires a different approach than models based on ODEs.

2.2 Interfaces to control and optimization tools

2.2.1 Polymerization process

Macro scale model was previously tested as a part of control tools, but a new experimental technique, Raman spectroscopy, enables a wider use of the model. Previously, only overall propagation constant could be estimated online (to reflect impurities in feeds), but now propagation constants for individual monomers can be estimated separately, which improves predictions of polymer properties.

Morphological model can be implemented as a part of control tools similarly as Macroscale model, because it is also implemented as a set of ODEs. In spite of a huge effort within the project, only partial success has been achieved in experimental techniques capable of online morphology characterization. Therefore, results of the morphology control can be robustly validated only offline after reaction. Efforts towards improved online morphology characterization and control are ongoing.

Implementation of Monte Carlo method into control tools is a bit tricky, because most methods usually employed for online control require models based on deterministic equations. Therefore, we implemented a surrogate model, which maps the space of control variables (temperature and monomer and initiator feedings) and replaces the local predictions of the Monte Carlo model by a continuous radial based surrogate function. An example of an interpolating surrogate function is depicted in **Figure 3**.

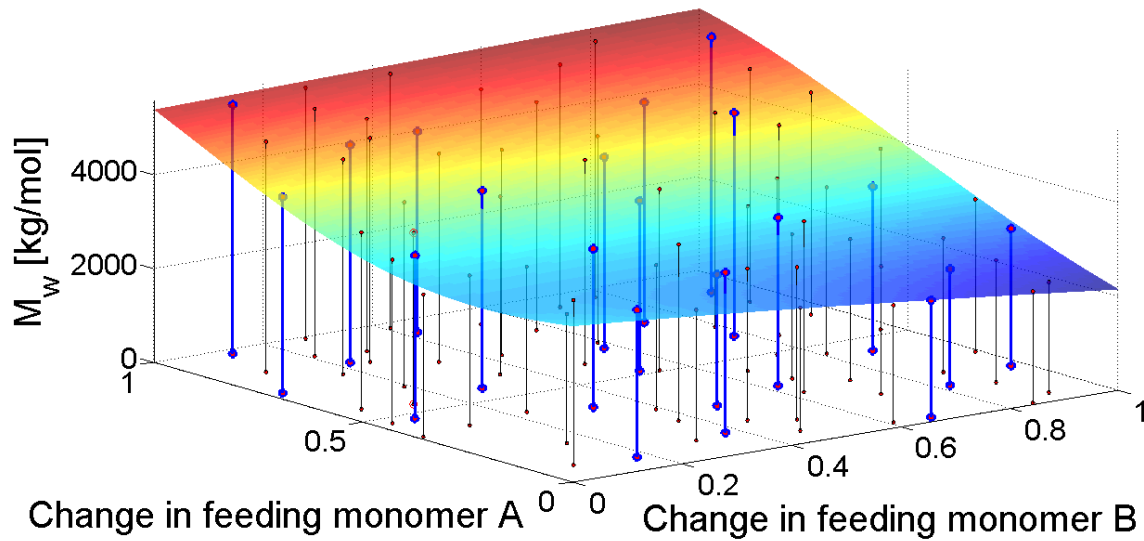


Figure 3: 2D intersection of the Monte Carlo predictions (dots on blue lines) and interpolated surrogate function (surface) respecting the statistical error of the Monte Carlo method.

Radial based surrogate function can be precomputed before its use in online control and automatically corrected in the most relevant positions during the control. This learning ability highly improves capabilities of surrogate function at not so well mapped conditions.

Implementation of surrogate modelling into a process control tools opens a huge possibilities not only for non-deterministic models, but also for models, which are computationally too demanding for online control.

2.2.2 Steelmaking process

The batch process chain for liquid steel production consists of four sub-processes, as already shown in Figure 2.

For each of the process steps σ in the steelmaking process route, an equation system is considered described by

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{f}_{\sigma}(\mathbf{x}_k, \mathbf{u}_k, \boldsymbol{\theta}) \\ \mathbf{y}_k &= \mathbf{h}_{\sigma}(\mathbf{x}_k, \mathbf{u}_k, \boldsymbol{\theta}) \\ \mathbf{0} &= \mathbf{g}_{\sigma}(\mathbf{x}_k, \mathbf{u}_k, \boldsymbol{\theta}) \end{aligned}$$

where $\mathbf{x}_k \in \mathbb{R}^n$ is a vector of state variables. Here state variables are the liquid steel temperature, and temperature of refractory-lined ladle and vacuum vessel. $\mathbf{y}_k \in \mathbb{R}^m$ are the measurements, $\mathbf{u}_k \in \mathbb{R}^d$ the inputs, and $\boldsymbol{\theta} \in \mathbb{R}^p$ the parameter vector. This model is approximated by a piece wise linear model as described by

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{f}_{\sigma(k)}(\boldsymbol{\theta}) + \mathbf{A}_{\sigma(k)}(\boldsymbol{\theta})\mathbf{x}_k + \mathbf{B}_{\sigma(k)}(\boldsymbol{\theta})\mathbf{u}_k + \mathbf{F}_{\sigma(k)}\mathbf{d}_k \\ \mathbf{y}_k &= \mathbf{C}_{\sigma(k)}(\boldsymbol{\theta})\mathbf{x}_k, \end{aligned}$$

with in this case a simplified automat

$$\sigma(k) = \begin{cases} 1 & \text{if } k_1 \leq k < k_2 \\ \vdots & \vdots \\ n & \text{if } k_{l-1} \leq k < k_l \end{cases}$$

where $\mathbf{u}_k \in \mathcal{R}^{d-s}$ is the control input and $\mathbf{d}_k \in \mathcal{R}^s$ is the part of the inputs which are not used for control but called disturbances. In the first step, the sums, products and quotients of parameters must be combined into one parameter. In a further step we determine with the help of the eigenvalue method which parameters are identifiable on the basis of the existing measurement data. The MPC and ILC have been designed on the basis of the identified model. The dynamic models described under 2.1.2 are used in the controllers for prediction.

The designed model, observer and controller are integrated in the tool shown in figure 4. It provides an overview of the BFI-ILC-MPC system and its interface to a typical Level 2 automation environment of a steel plant.

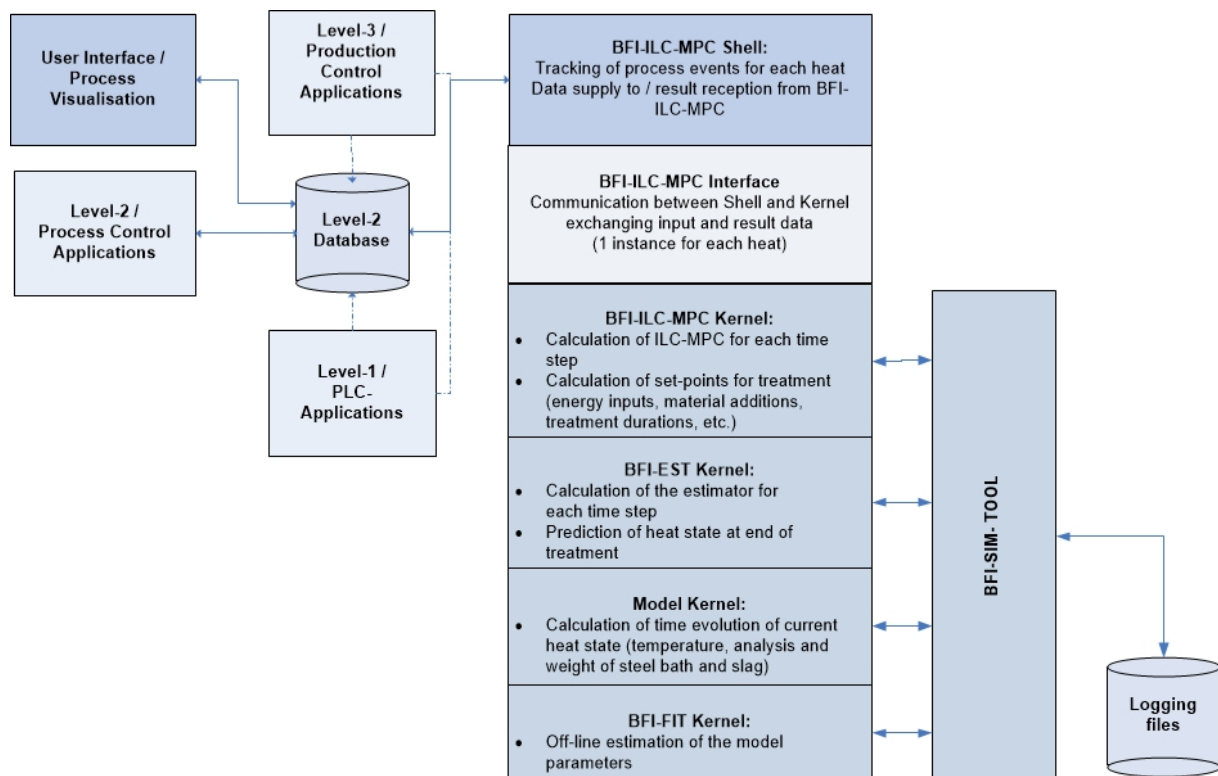


Figure 4: BFI-ILC-System overview

2.2.3 Silicon Production Process

There will be two versions of the model for the silicon refining process in the RECOBA project. The model RafSim described in Section 2.1.3 is an updated version of a previous process simulator, implemented in Python. This will be used for offline process simulations. The second version will be a reimplementation of this model in C/C++ and implemented and compiled as a Cybernetica CENIT model component and made suitable for online model based estimation and control.

The Cybernetica CENIT framework is illustrated in figure 5.

The model component to be developed for online use will communicate process data, measurements, estimates of states and parameters and derived outputs/controlled variables with the existing process control systems and database systems via the OPC communication protocol. OPC is chosen as a standard for RECOBA and will be the primary communication protocol used in the Silicon refining case. In the case of required data that is not available through OPC, a Windows Service will be created to acquire data from for instance a database and write it to an OPC-server. Cybernetica CENIT has built-in support for OPC communication and will be used in the implementation of the online model.

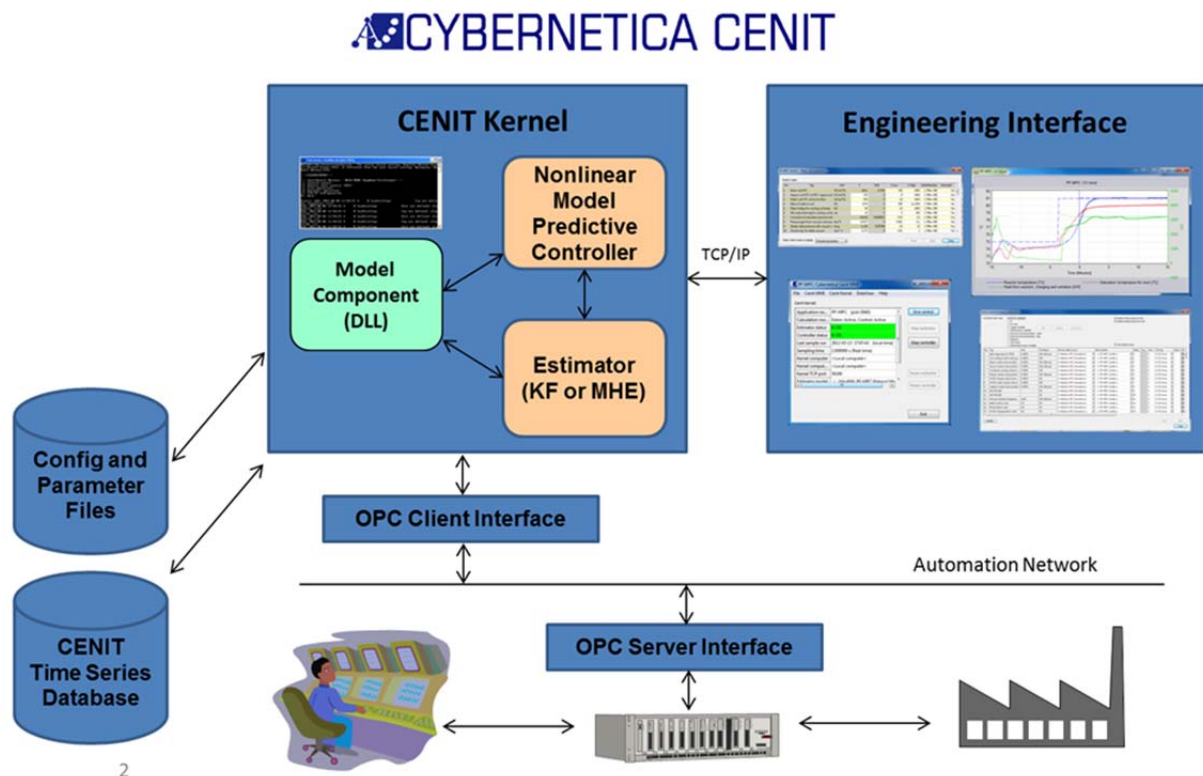


Figure 5: Illustration of the integration of CENIT into a process control system. The RafSim model is converted to a model component in CENIT.

The original version of RafSim has been available for some time and is roughly fitted to process data. This was done when the model was developed years ago, and a model fitting may have to be repeated now that a new model version is available. The online version of the model will be validated by comparing with the offline model as well as actual process data. Cybernetica Modelfit is a tool developed for model validation and parameter estimation either recursively or to one or several datasets. This tool will be used for the online model component.

The following measurements are available and in use in the refining process today:

- Chemical analysis
- Lip sample: A manual sample from the tapping streaming is performed approx. 1 ½ hrs after the tapping has started (20 min before the ladle is full).
- Dip sample: A manual sample from the ladle is performed 15 min prior to the ladle is full.
- Temperature in the melt.
- Ladle weight
- Ladle weight measured prior to start of tapping.

Sculls forming during tapping decrease the ladle volume and affects the temperature profiles of the ladle. The measurement should be included in the online model to estimate sculls for the current batch.

New types of measurements covered by RECOBA will be:

- Temperature monitoring of ladle refractories.

It is important to establish a correlation between sculls and refractory temperatures to be able to optimize the ladle temperature.

- Level measurements

A bath level measurement indicates the tapping flow into the ladle, which is important to maintain an accurate measurement of mass flow into the system, as well as serving as a safety measure in cases when increased sculling may cause the ladle to overflow.

The following actions are available for controlling the refining process:

- addition of slag-formers (silica sand, limestone/burned lime and alumina/aluminium metal),
- addition of solid Si (for cooling purposes),
- adjusting the flow of air/oxygen,
- adjusting the ratio of air to oxygen in the refining gas,
- refining time.

According to deliverable D 2.3, the process/control model of ladle refining should be able to predict the dynamic behaviour of the melt based on the following parameter groups:

- ladle geometry and stirring characteristics,
- slag (temperature, amount and composition),
- molten silicon (temperature, amount and composition),
- ladle refractories (temperature),
- metal flow from the furnace,
- eventual addition of slag fluxes and silicon (for cooling purposes).

The present offline version of the model can simulate the batch length of two hours within a few seconds. The present model is implemented in Python, which is an interpreted language. When the model is re-implemented in C/C++ it is expected to run faster, which means there is enough time for estimation and optimization for predictive control. The re-implemented online model will probably have some differences in the number of control volumes, and how these control volumes are configured. Some changes are likely to be made during the model development phase and when the online model is fitted and validated, but the main structure is predicted to be the same. At this point, there does not seem to be the need for model reduction, as the size and calculation speed of the existing model is appropriate for online use, and the suggested changes from the offline version to the online version do not significantly change this.

Process data gathered in WP 4.4 has been used for validating the process model described in Section 2.1.3. The model will be the basis for developing model-predictive control in WP5 to obtain the main goal of the RECOBA project in automating the refining process and decreasing the product quality variations.

Several plants today use a decision support system for follow-up of the refining process. The system calculates the suggested time for the final refining and the amount of additives added to reach the product specifications. The operators perform the corrective actions manually. By applying a validated model-based decision support system and direct on-line recordings of process parameters, Elkem anticipates that the yield of silicon will increase by several percent in the refining process, and that product quality consistency also improves.

The development of an optimisation tool assumes that key process data are available on-line. Elkem has accelerated the work of supplying this data to the on-line model. At Elkem Thamshavn, home to the largest Si-furnace in the world, gas flow and weight of solid additions to the process are now recorded automatically and made available to the on-line model. Further testing and improvement of the on-line model will continue after the RECOBA project has been finished.

2.2.4 Generalisation of interfaces to control tools for application at other batch processes

The previously given description of the control structure for the different batch processes again illustrates the similarities between liquid steel production and silicon refining. At both high-temperature processes continuous and direct measurements of the relevant process state variables (mainly temperature and composition of the melt) are not possible. Moreover, control actions in the process are only possible at certain times.

This presents an additional difficulty in both applications. In both cases, the control structure consists of an observer and a model predictive controller. The observer is event triggered in both cases, as the temperature measurements are not carried out in fixed time intervals. Due to the small number of measurements that are available online, on-line parameter estimation is not possible, but rather an estimate of the melt and ladle temperature.

Regarding the polymerisation process, the presented implementation of Raman spectroscopy in process control application enables an online estimation of more parameters than it was previously possible. In addition, the presented surrogate model, adapted online as required by control algorithms, provides fast predictions based on stochastic models. This application of surrogate models introduces a totally new concept of process control for complex processes.

3 Summary and conclusions

Summary and conclusions are provided separately for the different RECOBA use cases.

Polymerisation:

Several models were developed during the RECOBA project and a huge step forward was made for process control in complex situations. Application of Raman spectroscopy enabled online estimation of more model parameters than it was previously possible. Morphological models predict evolution of different phases in complex multiphase systems and thus enabled control of particle morphology in emulsion copolymerization. Hybrid Monte Carlo model revealed possibilities of developing stochastic models fast enough for online control. Overall the combination of continuous and stochastic modeling opens new possibilities in process control.

Steelmaking:

During the RECOBA project, a dynamic model for the entire process route of liquid steelmaking has been developed by BFI and validated with the help of process data

acquired directly at a steel plant. The analytical model is based on a mass and energy balance, involving thermodynamics as well as kinetics of the temperature relevant metallurgical reactions. The model focuses on monitoring and prediction of the melt temperature and is used in a slightly simplified version for real-time control applications, such as MPC and Iterative Learning control (ILC).

Silicon:

During the RECOBA project, an on-line model for silicon refining has been developed by Cybernetica and Elkem. The model accesses process parameters directly and predicts the composition and the temperature of the silicon melt in real-time. The physical model is built on fundamental principles such as mass and energy balance, thermodynamics as well as kinetics. This model is "re-engineered" using the Cybernetica software packages for real-time, on-line application.

Finally it was shown how the selected model structures and model interfaces to online process control systems can be transferred to other, similar processes within the process industry.