

## **CHALLENGE OF MODELLING OF HIGH-TEMPERATURE MATERIALS PROCESSES; OXYGEN CONVERTER PROCESS (LD, BOF) AS AN EXAMPLE**

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## **PROBLEMATIKA MODELOVANIA VYSOKOTEPLŔTNÝCH MATERIÁLOVÝCH PROCESOV; PROCES KYSLÍKOVÉHO KONVERTOROVANIA (LD, BOF) AKO PRÍKLAD**

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### **Abstrakt**

Výroba materiálov, napríklad výroba ocele, je veľmi komplexným procesom, v ktorom treba brať do úvahy transformácie rôznych látok a energie a zároveň aj trasportačné javy. V tejto práci sú vysoko teplotné procesy vnímané ako predmet modelovania a simulácie s cieľom vyhodnotenia riadenia procesov a tvorby programov. Všeobecnou podmienkou úspešnej simulácie je predpoklad, že všetky základné javy určujúce priebeh procesu môžu byť vzájomne prepojené a všetky chemické a tepelné zmeny v procese, počnúc vsádzkou až po vznik hlavných alebo vedľajších produktov prípadne aj odpadov môžu byť opísané s dostatočnou presnosťou v priestorových (kontinuálne, stacionárne procesy) alebo časových (vsádzkové procesy) súradniciach s použitím simulačných nástrojov rozličného pôvodu založených na rôznych princípoch. Opísané sú rôzne princípy a nástroje pre simuláciu vysoko teplotných procesov a takisto aj nevyhnutné podmienky a problémy kvantitatívnej simulácie. Ako príklad je použitý proces kyslíkového konvertorovania (LD, BOF). V práci sú vysvetlené hlavné javy nevyhnutné pre modelovanie tohto procesu. Okrem toho sú tu prezentované aj základné princípy fungovania simulátora kyslíkového konvertora CONSIM a niektoré výsledky získané simuláciou 55 tonového LD - konvertora v oceliarni Koverhar. Súčasťou práce sú aj nadobudnuté skúsenosti a problémy, ktoré sa vyskytli pri simulácii tak komplexného procesu ako je kyslíkové konvertovanie horúceho kovu.

### **Abstract**

Materials manufacturing like steelmaking processes are highly complex combinations of various matter and energy transformation and transportation phenomena. In this paper high temperature processes are looked as a subject of modelling and simulation for process control measures and programs. General prerequisite for successful simulation is that all essential phenomena controlling the progress of the process can be interconnected and the chemical and thermal progress of the process from the charge to the main and side products or wastes can be described with sufficient accuracy in spatial (continuous, stationary processes) or temporal (batch processes) coordinates using simulation tools of different principles and origin. Different principles and tools for simulation of high temperature processes as well as prerequisites and problems on "quantitative" simulation are discussed. Oxygen converter process (LD, BOF) is used as an example. The main phenomena essential in modelling of this process are described. Basic principles of CONSIM oxygen converter simulator and some results obtained with

simulation of 55 ton LD-converter at Koverhar steelworks are presented. Experiences and problems involving in simulation of such complex high temperature process as oxygen converting of hot metal are discussed.

**Key words:** high temperature processes, oxygen converting, LD, modelling, simulation

### Introduction

Processes, no matter if final or intermediate, aim to 1) products (like raw steel in LD-process used here as an example) and 2) side products or wastes (like slag & dust in LD-process) of optimal composition, temperature and minimum amount 3) with minimum expenditure of raw materials and energy 4) in minimum time by 5) maximum capacity 6) avoiding cardinal brakes in production. These goals can be seriously approached only with highly effective process control. Process control based on an exact physical model would be an ideal one but in a case of complex chemical processes like those used for high temperature production of steel and other metals and alloys this is not realistic. It is obvious that effective process control systems should be based on hybride models that are a combination of a *physical model* with *either statistical, fuzzy logic or neural network* methods for optimising data measured from the actual process and creating optimal models between the measured data and progress variables of the process.

### Phenomena in high temperature manufacturing and processing

Industrial chemical production processes are practically always heterogeneous the reaction system consisting of several phases between whom the chemical reactions, heat evolution/consumption and mass & heat transfer take place. Industrial processes are combinations of *matter and energy transformation and transportation processes*. Matter transformations are *physical* of their nature like changes in state: melting/solidification evaporation/condensation, phase transitions or more complex phase reactions, physical dissolution (like elemental gases in water) and physisorption or *chemical*: chemical reactions, chemical dissolution and chemisorption. In matter transformation processes there are always energy transformations involved – heats released or consumed in before mentioned matter transformation processes, *melting/solidification, evaporation/condensation, dissolution and chemical reactions* being the most prominent processes with relation to energy transformations, that should be necessarily taken into account in quantitative modelling and simulation of industrial processes. In a case of high temperature processes extra heat is necessary almost without exception as the charge materials have to be heated up to the reaction temperature. Heat is brought into the reactors either by burning fuel inside or outside of the reactor – in the latter case heat is transferred to the reactor by conduction through the walls – or transforming electric energy to heat inside the reactor by resistance or inductive heating. There are also energy transformations involved in remarkable volume changes in the reaction system. If only the volume change (of gases) against/by constant (outer) pressure takes place, energy changes are “automatically” included in enthalpy change in the reaction system.

Mass transfer proceeds through molecular level mass transfer mechanisms, *molecular diffusion, electrodiffusion* and by macroscopic mechanism, *convectonal mass transfer* (mixing in fluids). These two mechanisms are always combined in reaction systems comprising fluids. *Energy transfer* proceeds similar ways as mass transfer by atomic level *conduction* and macroscopic *convectonal heat transfer*. In addition there is radiation heat transfer that is the

more important the higher is temperature and its difference between the transmitting source and the environment.

Industrial processes are either *continuous, stationary* latter with no temporal but spatial changes inside the reactor or *non-stationary batch processes* with continuous changes in mass, energy as well as phase and compositional distribution inside the reactor. The progress of matter and energy transformation and transportation depends also on the technological principles of the process – co-current and counter-current reactors, top/bottom/side blown converters as examples. Different technological principles lead to different spatial and temporal characteristics of processes even if aiming to same products.

### **On the modelling of high temperature processes**

The ideal solution for modelling of processes is quantitative description of all matter and energy transformation and transportation processes inside the reactor and between the process and its environment as a function of time (*batch processes*) or reactor length (*stationary processes*). This is however hardly possible for actual production processes and we have to use combinations of physical models with models based on *statistical, neural network* or *fuzzy logic* analysis of various kind of data from the process.

Thermochemical processing is always a combination of matter & energy transformation and transportation processes. Whatever are the “true” physical driving forces for transformation and transportation processes at atomic or molecular level, *tendency to entropy production* and *gradients of thermodynamic potentials* (chemical/ $\mu$ , thermal/T and mechanic or pneumatic/p) relative to progress variables ( $\rightarrow$  transformation processes) or spatial co-ordinates ( $\rightarrow$  transportation processes) characterise all advancing processes and can be understood as their common and specific, local driving forces, respectively. A chemical process is an entity of driving forces and resistance for processes acting in the reaction environment, concerned. Driving forces tend to decrease with the progress of processes and when they all reach the zero value the reaction system has lost its ability to any kind of change and movement and the reaction system has obtained its equilibrium state. As the time available for the progress of industrial production processes is always limited, a “complete” equilibrium will never be reached in practice. An advancing chemical process undergoing matter transformation and transportation processes is always an inherently irreversible (An irreversible process in opposition to a reversible process is characterised by finite driving forces deviating from zero. Reversible processes are advancing from one equilibrium state to the next one, the driving forces of all material and energy transformation and transportation processes deviating only in infinitely small degree from zero) process, the entire process environment being characterised by non-uniform distribution of matter and energy within and between the homogeneous phases ( $\rightarrow$  gradients in chemical potentials of species, their concentrations, temperature and pressure).

The aims of traditional thermodynamic analysis of complex chemical or metallurgical processes are to define

- a final equilibrium state for the entire process or some of its specified zones;
- equilibrium conditions for some primary chemical reactions of the process;
- equilibrium distribution of some elements or species between the phases present in the reaction system;
- a reversible, through equilibrium states advancing thermodynamic reference process for the actual process (An irreversible process in opposition to a reversible process is

characterised by finite driving forces deviating from zero. Reversible processes are advancing from one equilibrium state to the next one, the driving forces of all material and energy transformation and transportation processes deviating only in infinitely small degree from zero).

### Hierarchy of modeling of metallurgical processes

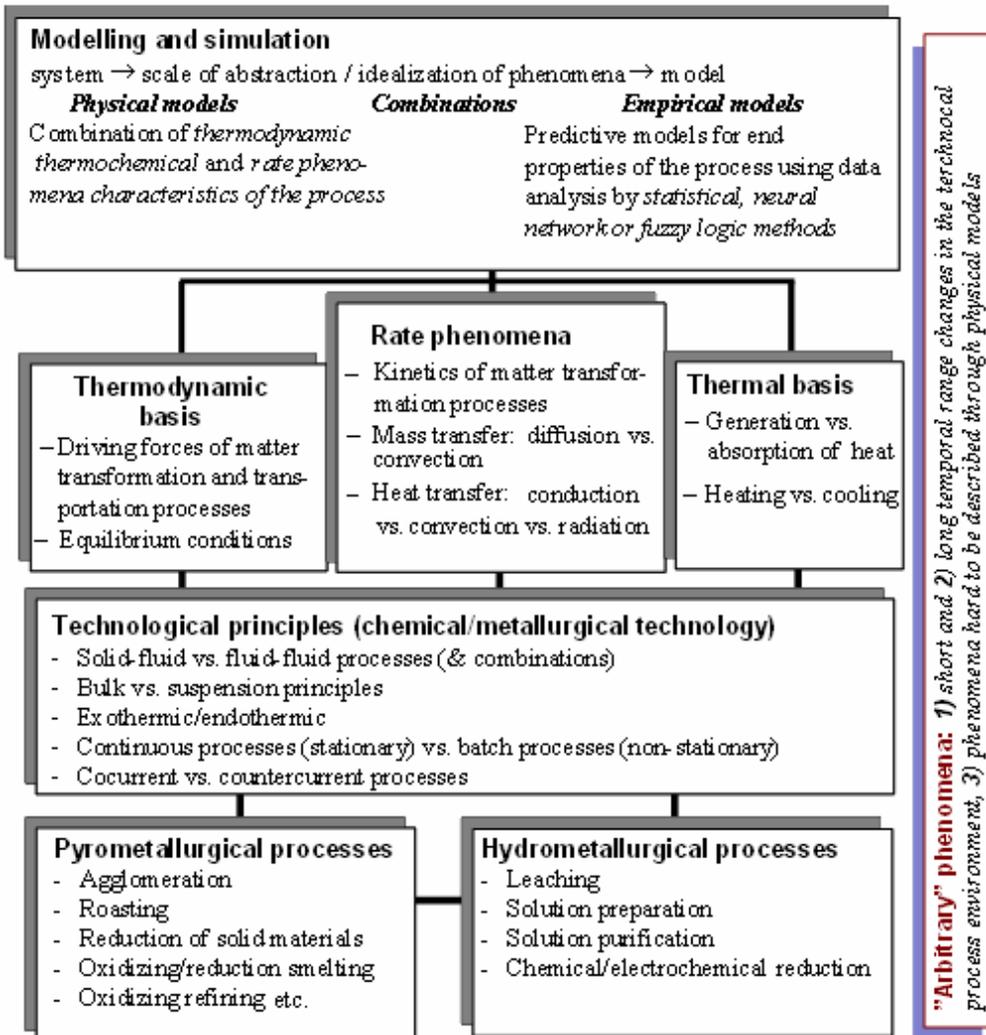


Fig.1 Hierarchy of modelling of industrial chemical processes (metallurgical processes as examples); Modelling and simulation by Lahiri [1]

It is important to keep in ones mind, that in actual processes thermodynamic (driving forces of matter transformation and transportation processes), thermochemical (energetics of the process) and rate phenomena (chemical kinetics, diffusion kinetics, fluid dynamics etc.) form an entity that control the progress of a process towards its equilibrium state. The classification of real processes to separate thermodynamic, energetic, rate phenomena and "arbitrary" or

“difficult to model physically” phenomena follows just from the necessity to simplify a highly complex set of real phenomena for process analysis. So called “conceptual analysis” or a conceptual model is the tool to evaluate relative importance of various phenomena for the final result of simulation.

Fig. 1 shows the hierarchy of aspects related to modelling of industrial metallurgical processes and Fig. 2 a procedure of creation of combined model through a conceptual model analysing the requirements for data and methods used for final simulation models.

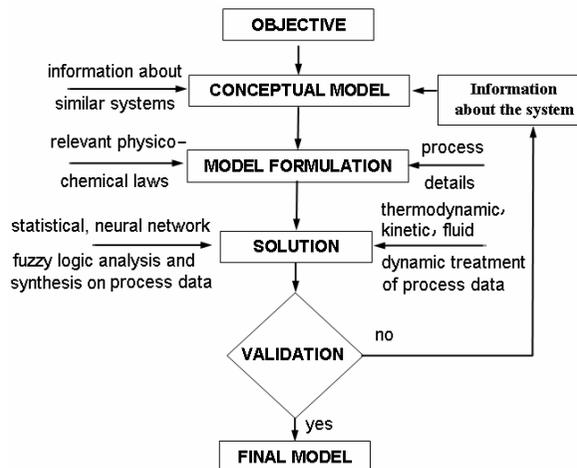


Fig.2 Flow chart of (conceptual) process modelling –slightly modified from Lahiri’s presentation [1]

### Oxygen converter process as an example for process simulation

Oxygen converter processes like LD-process and its further modifications are batch processes in which from 50 to +300 ton of hot metal from blast furnace is oxidising refined to raw steel (Fig. 4). In a LD-process carbon and other minor hot metal constituents like silicon are oxidised to desired level blowing oxygen onto the surface of iron melt. Modern LD-converters are provided with bottom tuyeres for enhancing mass transfer in iron melt by inert gas blow.

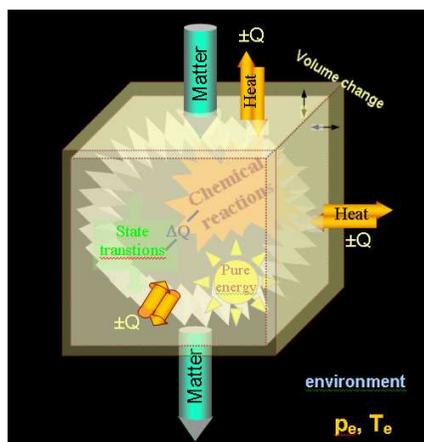


Fig.3 A principal scheme of an industrial process with matter and energy transformations and transportation processes. The inner volume (dimensions), mass flow conditions inside the reactor as well as heat transfer characteristics through reactor walls will change with total processing time in high temperature reactors.

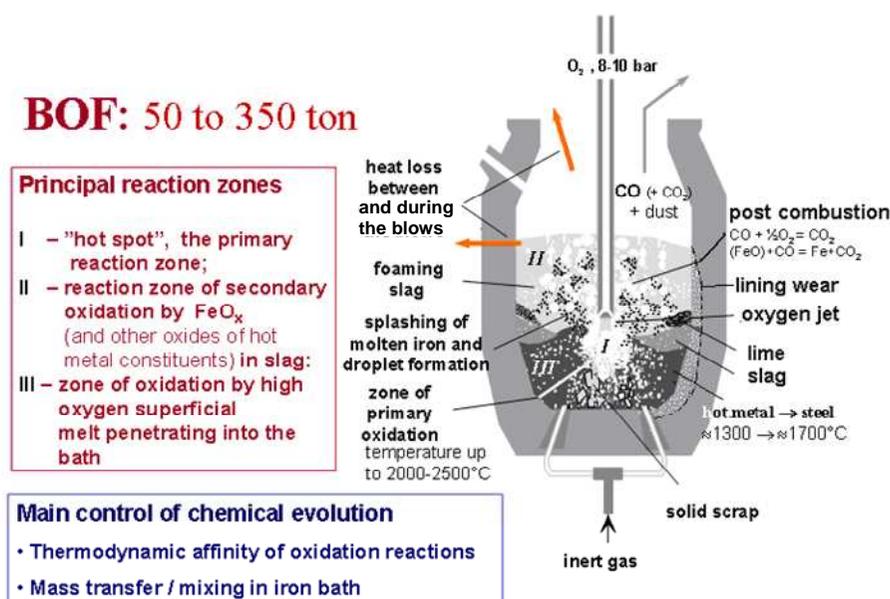


Fig.4 A scheme on LD-process with inert gas bottom stirring as an object of modelling

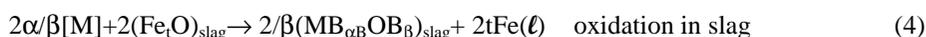
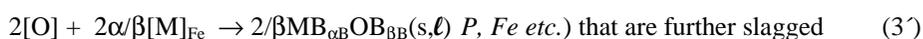
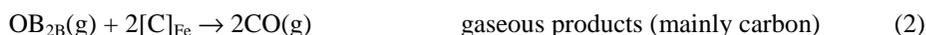
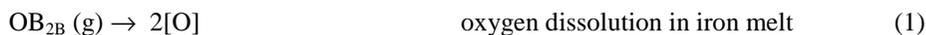
Charge comprises besides hot metal usually slag formers, lime or doloma, scrap as coolant and as additional iron source besides hot metal, sometimes also fluorspar, sinter (ore) and extra fuel like coke or ferrosilicon. The most important target values are the *end carbon content* and *end temperature* of steel. Carbon content of hot metal is around 4 wt%, silicon, titanium, manganese, vanadium and phosphorus contents are few tenths of percent or even less than one tenth (P, S). The minor constituents and some iron are oxidised and slagged, except of carbon that leaves the reactor as gaseous oxides, mainly as carbon monoxide. Some amount of scrap (usually 10 -20% of hot metal charge) is melted by the heat released in highly exothermic oxidation reactions.

In primary oxidation of carbon in hot metal the major product is carbon monoxide that is partly oxidised by primary oxygen above the surface of iron melt and by oxides in slag when passing the foamy slag – this phenomena is called as *post combustion*. Heat produced in highly exothermic chemical reactions (primary and secondary reactions like post combustion) is consumed in heating up the charge materials like slag formers, coolants and scrap that is melted, as well as iron melt (from the initial hot metal temperature, usually  $1300\text{C} \pm 50^\circ\text{C}$ ), slag and off gas. Some part of the condensed charge materials and products escapes the reactor with off-gas in the form of dust.

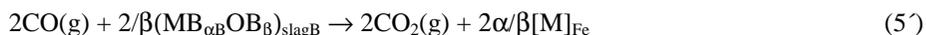
The main phenomena in oxygen converter process are oxidation of hot metal constituents with heat evolution. Oxidation reactions comprise as a whole following steps:

- 1) fluid flow mass transfer of oxidising elements to the the superficial layers of iron melt where primary oxidation proceeds
- 2) circulation transfer of iron droplets in slag
- 3) diffusion on oxidising elements to oxygen/melt and droplet/slag interphases
- 4) chemical act at gas/iron melt, slag/iron droplet and CO-bubble/slag interphases

Oxidation reactions take place in three main reaction zones, on oxygen blow impingement surface, inside the iron melt between high oxygen iron from impingement surface mixing with low oxygen high alloy element iron from bath interior and between iron melt droplets circulating in slag (see Fig. 2). The oxidation reactions are, accordingly, of following types



Slag forming is a compilation of several steps where oxides from various reaction environments react with lime or dissolve in molten slag. Post combustion reactions are of following types



In addition there is evaporation of iron and some hot metal constituents (especially at hot spot in the oxygen jet impinging the iron bath surface

Heat brought into the converter by molten hot metal and evolved in chemical reactions is transported inside the iron and slag melt by fluid flows (mixing) and further evened out by conduction. It is mainly consumed in

- 1) warming up and melting the cool charge components especially scrap heating and melting
  - 2) heating of iron and slag melts in the converter or
  - 3) escaped from converter by off-gas and dust as well as
  - 4) by conduction through the furnace walls and also by radiation from reactor lining especially during the charging period
- < 5) endothermic chemical reactions >

Simulation aiming to quantitative description of chemical and thermal evolution of the process - in the case of oxygen converter process simulation aims to suggestion for 1) charge composition, 2) blowing program (blow rate, lance height program), 3) total oxygen consumption and blow time, leading to desired blow results, desired carbon content and temperature of raw steel. Simulation should comprise all major matter and heat transformation and transportation processes listed above. These phenomena could be at least in principle included in a physical model. In addition there are some important phenomena that are not easily included in a physical model like heat losses to the reactor environment during and between the blows, post combustion degree and post combustion heat distribution between the melts and off-gas, dust formation, lining wear affecting the melt area and heat loss, wear of tuyere openings

and such fully arbitrary phenomena like skull formation on the mouth area of the furnace and on oxygen lance that could effect the flow pattern in the converter.

*Basics, experiences and problems on oxygen converter simulation, CONSIM-simulator*

The basis of oxygen converter simulator CONSIM [2, 3, 4, 5, 6, 7, 8, 9, 10] is the central reaction module that includes model for oxygen distribution in oxidation reactions and mass transfer model which together control the progress of primary oxidation(/reduction) reactions. In this module three reaction environments are substituted by one generalised reaction zone. This module computes the progress of all basic chemical reactions as a function of oxygen consumption. Mass transfer model is a combination of diffusion and convective mass transfer. This simplification is dictated by the fact that modelling of three discrete reaction zones changing matter and energy with each other is far to complex to model especially without detailed quantitative knowledge of matter transformation and transportation processes. The principle of central reaction module or model is presented in Fig. 5. Besides the “central reaction module” for oxygen consumption and primary oxidation reactions, there are several sub-models computing *scrap melting, lime dissolution, post combustion, dust formation, slag reduction and heat loss* during and between the blows in connection with the progress of main chemical and heat release in them.

In Figs. 7, 8 and 9 an old blow in Koverhar steelwork's 55-ton LD-converter (Fig. 10) is simulated. Due to lack of exact information on the charge, blowing program and end temperature for the actual blow, simulation is only approximate showing however similar behaviour of hot metal element oxidation. Exact information about the end temperature of steel for the actual blow was not available, only an estimate for target temperature that was slightly over 1700°C.

In simulation the effect of silicon diffusivity on the progress of silicon oxidation rate was also tested as an example of the problems caused by differences in basic data used for the physical model. For silicon diffusivity there is large variation in values reported in literature. As can be seen when comparing Figs. 7 and 8, a change in silicon diffusivities by 100-fold (difference in silicon diffusivities given in literature) affects silicon oxidation rate, slightly also the end temperature and slag iron content in simulation. Changing the values in thermodynamic and diffusion databases or parameters in various subprograms (heat loss, post combustion, dust formation etc.) will cause changes in simulated steel composition and temperature. For example the choice of standard thermodynamic data for iron oxide “FeO” (in literature there is data available for various stoichiometry:  $\text{Fe}_{0.945}\text{O}$ /  $\text{Fe}_{0.947}\text{O}$ /FeO) and partial molar properties in slag melt (activity coefficient  $\gamma_{\text{FeO}}$  as a function of temperature and slag composition) has a great effect on iron oxidation and end temperature, but only in a case of low carbon steels corresponding to high oxygen potential/activity in the end of the blow. This makes the assessment of various parameters as a very problematic task especially, when the information from actual blows is limited as usually.

Fig. 10. shows simulation results for 21 high carbon steel blows in Koverhar steelwork's 55 ton LD-converter from year 2000, when the reactor was not yet provided with bottom blowing facilities, compared with the actually measured values. Although the results of simulation follow the tendencies shown by measured values and are on right level the scatter is quite high. The reason is partly in inaccuracy in some measured data and lack of some important

data, but also on the fact that a physical model extended with simple mathematical models for part of the phenomena in the process (mainly post combustion and heat loss models) using *non-sophisticated methods for parameter optimization*, is not accurate.

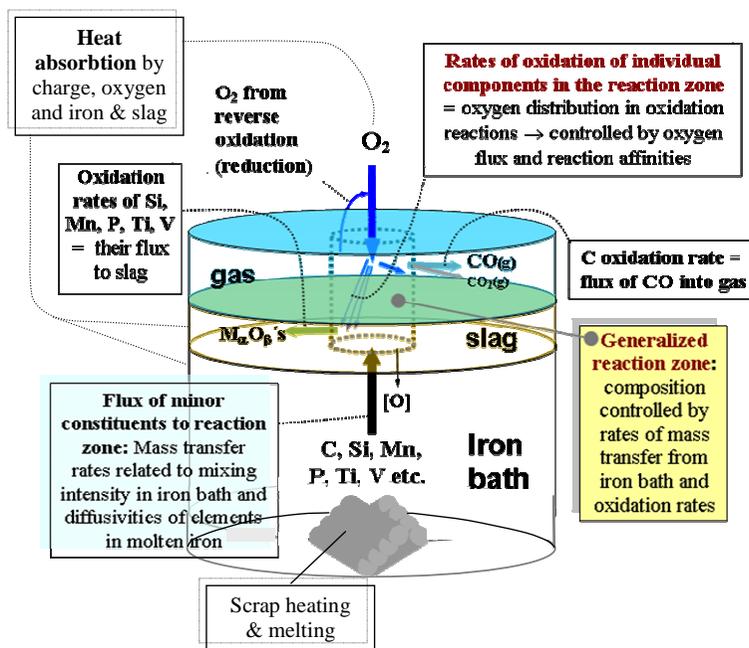


Fig.5 Principal components of a central reaction module with sub-modules for heat absorption by molten phases and consumption in scrap melting.

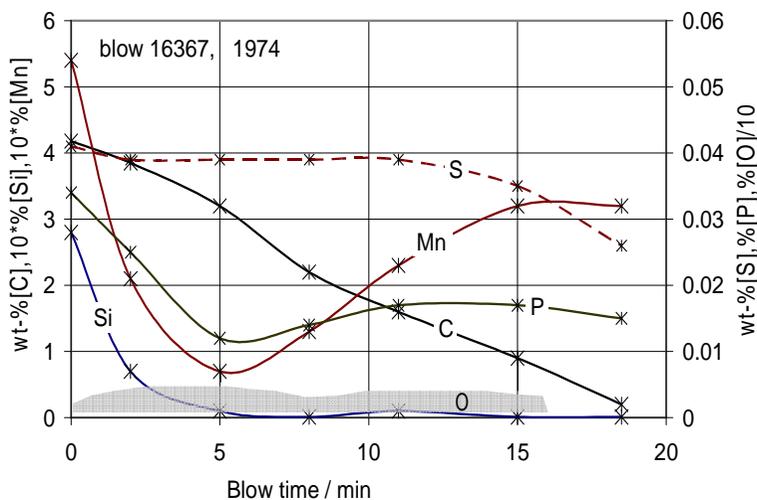


Fig.6 Change of iron melt composition in a blow at Koverhar steelworks simulated in Figs. 7 and 8. Iron oxide content in slag expressed as stoichiometric FeO was 25 wt-%.

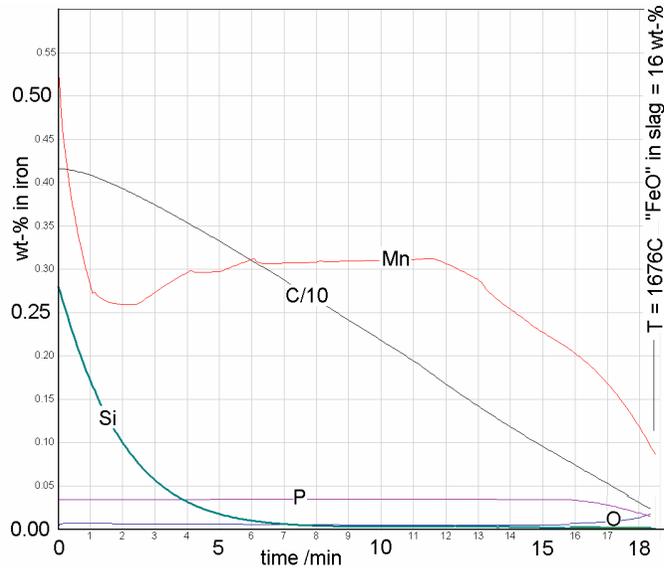


Fig.7 Chemical evolution of iron melts in simulated blow in 55-ton LD-converter of Koverhar steelworks. (silicon diffusivity in simulation =  $5 \cdot 10^{-8}$  cm<sup>2</sup>/s).

The comparison of effect of different silicon diffusivity values was presented just to emphasise the role of basic data as there are in literature sources available differing values or functions. This concerns as well the thermodynamic and thermal data, especially partial molar properties (activities and heats of solution) of species in solutions but also data for pure stoichiometric species.

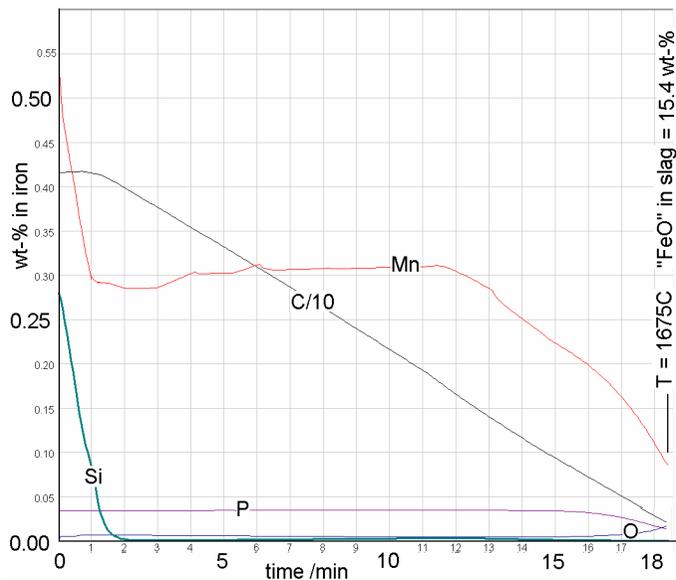


Fig.8 Chemical evolution of iron melt in simulated blow in 55-ton LD-converter of Koverhar steelworks (silicon diffusivity in simulation =  $5 \cdot 10^{-6}$  cm<sup>2</sup>/s).

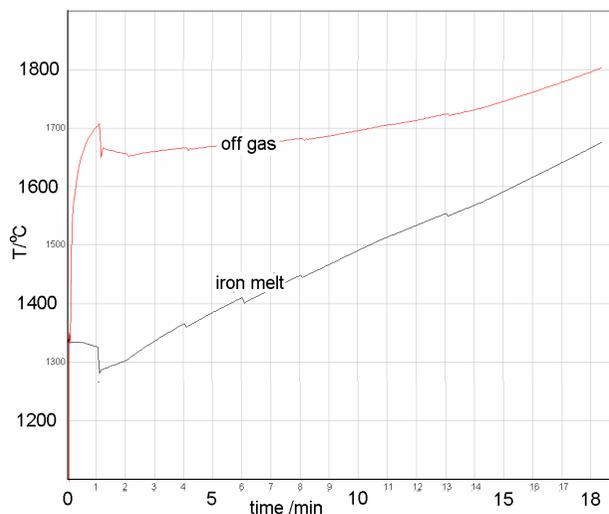
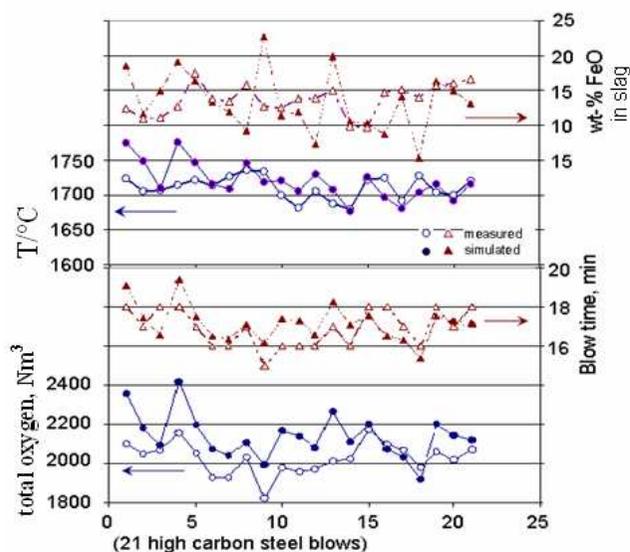


Fig.9 Thermal evolution of iron melt in simulated blow (silicon diffusivity =  $5 \cdot 10^{-6} \text{ cm}^2/\text{s}$ ).



#### Average data of 21 high carbon steel blows at Koverhar steelworks

	Blow rate $\text{Nm}^3/\text{min}$	Lance height m	wt% C	Scrap ton	Converter dust + ore ton	FeSi ton	Lime ton	CaF <sub>2</sub> ton
<b>High C</b>	120	1.15	0.686	2.15	1.05	0.099	3.15	0.31

Fig.10 Results of simulation some final properties of 21 high carbon steel blows in Koverhar 55-ton converter by CONSIM 5.1

#### Concluding comments

It is obvious that for quantitative simulation of complex high temperature processes the right choice is to build the program on a physical model extended with empirical models for

such phenomena that cannot be described by a physical model. The combination of physical and empirical models just gives a qualitatively right interdependence between the properties required for process control and input information as well as the measures to control the process such as top and bottom blow parameters. One series of problems is how to take into account the role of mole or less arbitrary phenomena like slow "ignition" of top blow, big variation in blowing rhythm (affecting heat content and temperature of furnace lining), splashing of melts from reactor, "overfoaming" of slag, (uneven) wear of furnace lining, skull formation etc.

Conditions prevailing in converter during a blow are very dynamic and might change with the progress of a blow. Temperature distribution is very uneven. In "hot spot" it is reported to be observed temperatures up to 2500 – 2600°C. This for sure affects the evaporation of iron and some other iron melt constituents i.e. on dust formation but also heat radiation to the direction of converter mouth. It is very obvious that in hot pot everything is oxidized and one can ask, what is the stoichiometry of iron oxides and other oxides formed at the hot spot. Both phenomena are further greatly affected by the state of slag – if there is foaming slag absorbing both heat and evaporation products or non-foaming viscous slag.

One general problem in simulation of actual converter blows is the accuracy of data from individual converters necessary in construction of the models and in assessing the model parameters and even in creating of a conceptual understanding on the importance of various phenomena within the process.

Due to high complexity of the LD-process, pure physical simulation alone with additional simple empirical models for phenomena that are not suitable to be presented as physical models, is not capable to produce high enough accuracy. Application of such effective methods like neural network for assessing the parameter in the physical models simulating the progress of major matter transformation and transportation processes and in supporting empirical models would be of important aid in increasing the accuracy of simulation. But everything should be started with establishing a conceptual model for the entity of phenomena in order to choose only those phenomena that are necessary in creation of proper combination of sub-models that gives accurate enough results of simulation and helps to avoid overmodelling.

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