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MATHEMATICAL MODELLING - AN INTEGRATED PART OF ELKEM'S CONTINUED EDUCATION FOR PROCESS METALLURGISTS

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ABSTRACT

The stationary/average behaviour of the (ferro)silicon process has been described by a comparatively simple stoichiometric model. The process is divided into a hot hearth region and a comparatively colder upper zone. In the hearth energy is supplied, and silicon is produced along with the crater gases SiO and CO. In the upper zone a large part of the SiO-gas is recovered, either by converting carbon to SiC or by "condensing".

The stoichiometric model is now an integrated part of Elkem's continued education for the process metallurgists within the frame of The Elkem University. In the special sessions for the FeSi/Si-processes, theoretical lectures alternate with hands-on model sessions.

The stoichiometric model and its educational use have established a common basis for exchanging theories, ideas, and experience among Elkem's research specialists and process metallurgists.

INTRODUCTION

It is not easy to envision what exactly is going on inside a ferro-alloy furnace. Interpretations from metallurgists have often diverged, giving rise to the old saying: "Wherever two or three metallurgists are gathered, you will find at least four opinions on the process conditions." Looking at the process one will find more than one reason for such a lack of consensus:

- The main part of a ferro-alloy process occurs in the middle of the furnace, in an extremely hot hearth region, inaccessible for direct observations. Single observations on for instance the furnace top are insufficient for determining the conditions in the hearth.
- The dynamics of the process are quite complex with time constants (response time) ranging from less than a second (some electrical phenomena) to several days (months or even years for the extreme cases), and the furnace never seems to be in a steady state.
- There has often been a lack of proper communication between research metallurgists (with good theoretical knowledge) and process metallurgists (who know how to handle the everyday problems).

It is clearly a drawback when the process is sufficiently obscure to foul (even) experienced metallurgists. Improvements have, however, been achieved due to:

- Systematic research for improved process understanding
- Improved instrumentation and automatic process control
- Proper training and continued education for operators and metallurgists

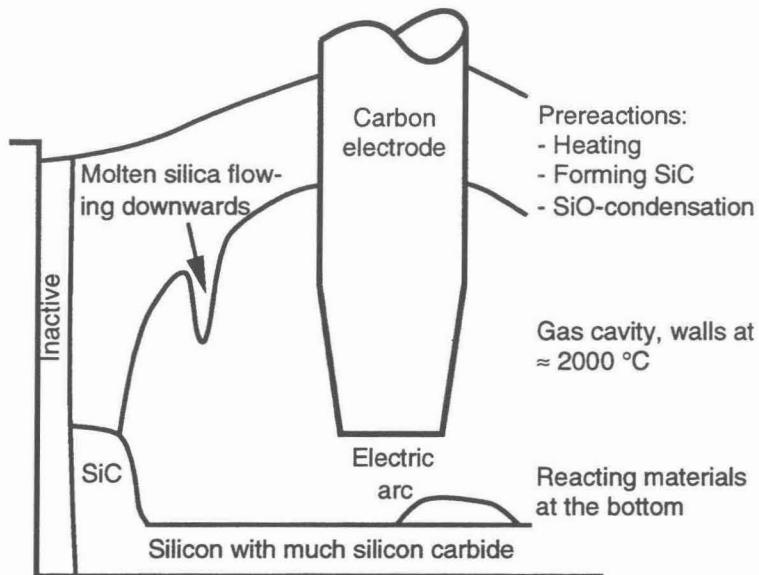


Figure 1 - Active zone of an operating (ferro)silicon furnace. The cavity is exaggerated.

During the last years the latter has been highly emphasised within Elkem. For some time mathematical modelling has been an integrated part of Elkem's research on improving our process understanding for the (ferro)silicon process. It turned out that one of our models was also an excellent tool for educational purposes.

MODELS FOR THE (FERRO)SILICON PROCESS

The (ferro)silicon process

The (ferro)silicon process was developed empirically. After 1892 the French chemist Moissan treated a variety of materials in his electric arc furnace. The combination of quartz, iron ore and carbon gave a useful product, ferrosilicon, and the process was transferred to a production plant. The scale of the operation has increased steadily, and furnace construction and the auxiliary systems for transport, weighing and control have been modernised, but the basic process is essentially unchanged.

The process is normally carried out in large three-phase electric furnaces. A simplified picture of the inner structure of the silicon submerged-arc furnace is shown in figure 1. A gas filled cavity is formed around each electrode tip, and the final reactions run on the sides and at the bottom of the cavity. The main part of the heat is evolved in electric arcs beneath the electrodes.

The process is normally run in cycles. During operation the cavity increases as the charge materials are consumed. The material layer above the cavity becomes increasingly thinner and hotter. Gradually it becomes white-hot, and smoke-containing gases escape. At last the top layer breaks down or is stoked down, and new materials are added at the top. Then the cycle is repeated.

The chemical reactions within the (ferro)silicon furnace were not investigated for many years, and as late as in 1950, they were practically unknown. At this time the management of Elkem started a research programme*) at the Norwegian Institute of Silicate Research with K. Motzfeldt as the main scientist. He proposed a simple stoichiometric model for the process. This model has been further developed and was finally implemented on Excel spreadsheet in 1991 [1,2].

*) To our knowledge other companies have carried out similar programmes, without publishing the results.

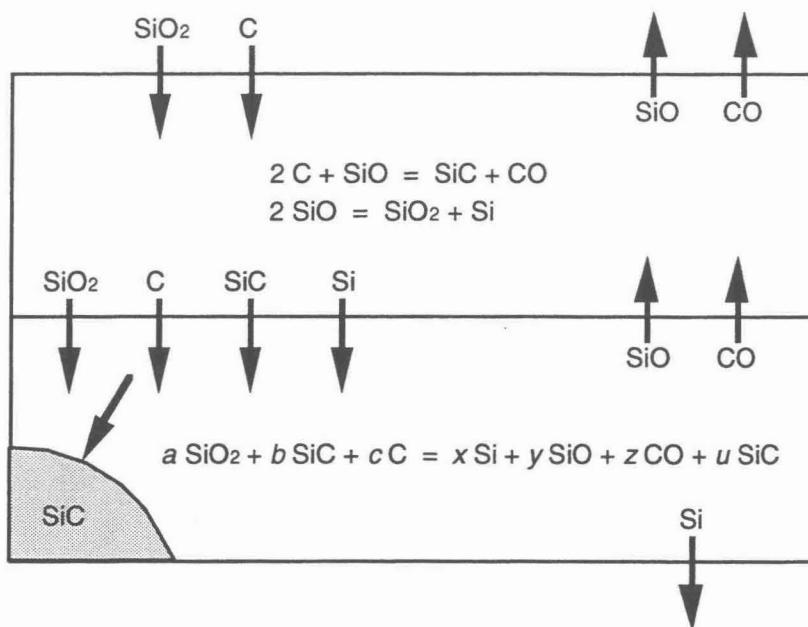


Figure 2 - Simplified picture of the stoichiometric model

To further improve the process understanding a unidimensional dynamic model has also been developed to take into account the dynamic interaction between energy supply, reaction kinetics, heat and mass transfer [3,4,5].

As a simplification, Elkem's models for the (ferro)silicon process do only treat pure silicon produced from a charge of pure raw materials (SiO_2 and C). As the silicon chemistry is dominating, the models apply, however, to the production of silicon and iron-silicon alloys containing from about 60 to 100% Si.

A stoichiometric model

In Elkem's stoichiometric model the average stationary state of the silicon process is simulated. For the model the following fundamental elements are considered/included:

- Thermodynamics
- Kinetics
- Material balance
- Heat (energy) balance

Thermodynamic studies show that the hearth of a silicon producing furnace must be hot (above 1811 °C*) and contain a high amount of SiO -gas (approximately 50 %, the remaining gas being mainly CO). To get a reasonable silicon recovery (corresponding to normal industrial practice) a large part of the SiO -gas must be recovered as the gas passes through the upper parts of the furnace [1]. Hence, a model of the process must include an inner hearth zone, where Si can be produced, and an outer "cold" zone, where SiO -gas can be recovered. To stay simple, a first model only includes these two zones as shown in figure 2.

*^o) Triple-point for coexistence of SiO_2 , SiC , and Si at 1 bar estimated with the most recent data from JANAF Thermochemical Tables [6].

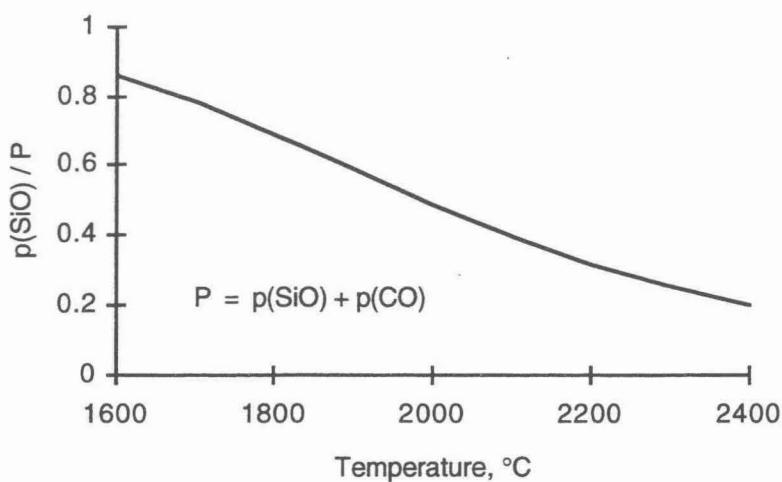


Figure 3 - The equilibrium $\text{SiO(g)} + \text{SiC(s)} = 2 \text{Si(l)} + \text{CO(g)}$ calculated with data from JANAF Thermochemical Tables [6].

Thermodynamic studies will also show that only the components C (solid), SiC (solid), SiO_2 (solid/liquid), Si (liquid), CO (gas), and SiO (gas) can exist in significant amounts in the temperature range relevant for a silicon producing furnace (when only pure raw materials are considered).

The equilibrium condition for the formation of free Si is given by the reaction



The equilibrium is shown in figure 3. Points below the curve correspond to conditions where free Si is unstable. This defines a minimum content of SiO in the gas for formation of silicon. In the process there is a (more or less continuous) supply of materials to the hearth, and the equilibrium for reaction (i) can not be completely achieved, due to kinetic restrictions. In the model we treat this by stating that the gas produced in the hearth of the furnace is characterised by a (thermodynamic/kinetic) parameter s such that:

$$\frac{p_{\text{SiO}}}{p_{\text{tot}}} = \frac{p_{\text{SiO}}}{p_{\text{SiO}} + p_{\text{CO}}} \geq s \quad (\text{1})$$

This s is assumed to be constant for a given charge and a given mode of operation.

Let a , b and c be the flows (in moles/s) of SiO_2 , SiC, and C to the hearth. Then the overall conversion in the hearth can be described by:



The material balances for Si, C and O supply three equations for the four unknown coefficients x , y , z and u . To get a fourth equation, we utilise the fact that the ratio between the gas pressures must be equal to the ratio between the gas flows. The restriction (1) can then be rewritten as a linear inequality:

$$\frac{p_{SiO}}{p_{SiO} + p_{CO}} \geq s \Leftrightarrow \frac{y}{y+z} \geq s \Leftrightarrow s(y+z) - y \leq 0 \quad (2)$$

The equation system can now be solved, when requiring non-negative values for the unknown coefficients in (ii). Depending on the input flows to the hearth, we get either [2]:

- a true stable solution with no SiC build-up ($u = 0$), where the SiO-pressure generally is higher than the limit given by (1).
- a solution where SiC is deposited in the hearth ($u > 0$), and the SiO-pressure is given by equality in (1).

On the basis of measurements in small scale furnaces [1], a hearth temperature of 2300 K is assumed. The heat (energy) balance can then be used to compute the energy requirement. The main effect of altering the hearth temperature is changing the equilibrium conditions for equation (i). This can still be simulated in the model by adapting the s -parameter.

In the outer zone capturing SiO is the important aspect. At temperatures above 1514 °C*) the thermodynamically preferred reaction is [1, 7, 8]:



This reaction soon forms a carbide layer on each C-particle, which slows down further conversion. From practical experience it is also known that carbon materials often do not react completely. We have therefore defined a reactivity number, r , which specifies the fraction of carbon that will react according to (iii), provided a sufficient amount of SiO is available.

If SiO is cooled down, it will start to "condense". Experiments show that the main reaction is [7, 8]:



This reaction is strongly exothermic, and the released heat will raise the temperature of the incoming raw materials.

Reaction (iv) will run in a temperature range about 2000 K. To simplify calculations, the model assumes that the raw materials are first heated to 2000 K, and then react at this temperature, before the (intermediate) products are transferred to the hearth zone. The heat balance is applied to compute the amount of SiO that will condense.

To sum up: In the hearth region the thermodynamic and kinetic requirements are fulfilled by assuming a suitable temperature and requiring that the SiO pressure is above a certain limit. Material balances are utilised to solve for the material flows/conversion, while the heat/energy balance is used for computing the energy requirement. In the upper zone the material balances are fulfilled by only letting (a few) balanced reactions run. A thermodynamic restriction is to let SiO escape only at a high temperature. The amount of SiO that "condenses" is found by using the energy balance, assuming reactions running at 2000 K. A kinetic restriction is included by assuming that only a specified fraction of the carbon can be converted to carbide in the upper zone.

*) Triple-point for coexistence of SiO₂, C, and SiC at 1 bar estimated with the most recent data from JANAF Thermochemical Tables [6].

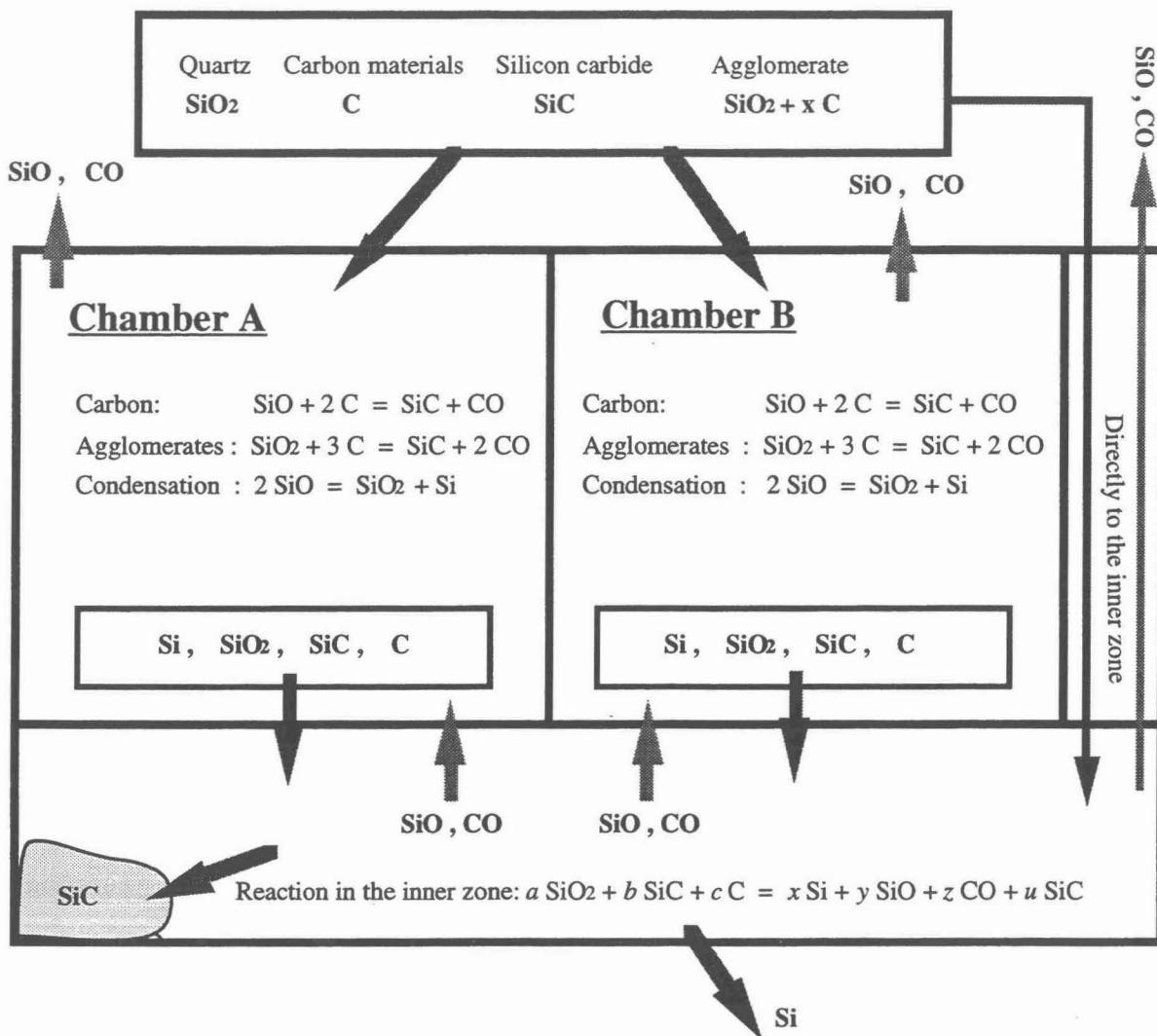


Figure 4 - The stoichiometric model with reactions and material flows

Basically the model is a two zone approximation as described above. The model has, however, been further expanded by splitting the upper zone into two chambers A and B as shown in figure 4. This splitting was suggested by Kolbeinsen [9] as a method for simulating imperfections in the counter current between the incoming charge and the outgoing gas. The distribution between the two chambers can be chosen at will both for the charge at the top and for the gas from the inner zone. In addition, charge materials can be added directly to the inner zone, and gas can be removed from it without interfering with materials in either chamber. The charge can consist of SiO_2 , C, SiC and mixed agglomerates [$\text{SiO}_2 + x \text{ C}$]. The complete model is described in further detail in [2].

To find the overall conversion for the whole furnace the equations in the hearth and in the shaft must be solved simultaneously. In our implementation this is done by iterations. Assuming a certain SiO_2 - and CO-flow from the hearth, the conditions in the upper chambers are first solved, supplying the necessary material input to the hearth. The hearth equations can then be handled. Afterwards a new iteration can be performed based on the (latest) computed gas flows from the hearth solution, etc. The process is repeated until converging within a sufficient accuracy.

The model is implemented in Excel. Most of the calculations have been entered in a normal spreadsheet. The iterations, input checks, dialogues, and some special evaluations have been programmed as Excel macros.

A unidimensional dynamic model

The dynamics of the process are complex, and the state of the process can easily be misinterpreted if the dynamic behaviour is not understood. Our dynamic model addresses this problem. The model has been developed to study both short term dynamics (variations within the stoking cycle, extreme short term electrical phenomena are not included) and long term dynamics (days, weeks or more).

Compared to the stoichiometric model the dynamic one is rather complex. Not only dynamics are included, but also variations in the height direction. Thermodynamic equilibria for the reactions involved are included (which means that for instance the temperature variation in figure 3 has been implemented). The chemical kinetics are described by rate laws where the reaction rate is proportional to the (local) deviation from equilibrium. The input parameters in the rate laws are separate for each reaction, and the direction in which the reaction is running. (Reaction (iv) is for instance fast when SiO condenses and seems to be slow in the opposite direction.) The material and heat balances are formulated as differential equations, which have been spatially discretized and are then integrated numerically by a suitable time stepping algorithm.

Through case studies it has been shown that the stoichiometric and the dynamic models are consistent, i.e. both models predict (qualitatively) the same stationary behaviour. Due to its simplicity it is extremely easy to perform series of computations with the stoichiometric model. On the other hand: the unidimensional model supplies dynamic information, and in addition more detailed process insight due to its finer structure and more realistic descriptions (as opposed to the lumped parameters r and s , which accounts for several effects in the stoichiometric model).

The dynamic model is thoroughly discussed in [4] along with a comparison of the two models. A comprehensive presentation of the model equations can be found in [5].

CONTINUED EDUCATION FOR PROCESS METALLURGISTS

The Elkem University

Increased productivity in ferrosilicon production was the operational objective for the research project FeSi 8000, where improvements were achieved by merging furnace experience with research effort. Among the important spin-offs from the project were educational programmes, both for operators and for process metallurgists [10].

The course for the process metallurgists has been organised as an up-grading course within the frame of The Elkem University. The first course in 1991 was only for the FeSi/Si-processes. It was an immediate success, and the following courses (1992, 1993, 1994, ...) also included Elkem's Mn- and Cr-processes, with partly common sessions and partly separate/parallel session depending on the topics.

The courses that have lasted for two separate weeks, have focused on process theory at university postgraduate level. The course in 1994 was actually arranged in co-operation with The Norwegian Institute of Technology in the format of an ordinary Continuing Engineering Education Course (but not open for general participation), with the option of examination and university course credits.

Topics that have been covered include process theory, raw materials, process models, simulation studies, electrical conditions, Søderberg and prebaked electrodes, control theory, statistics, furnace economy, basic thermodynamics, and heat transfer. Some of the issues (e.g. statistics and basic thermodynamics) have not been covered at each course. Lecturers have been from Elkem and from external sources such as The Norwegian Institute of Technology.

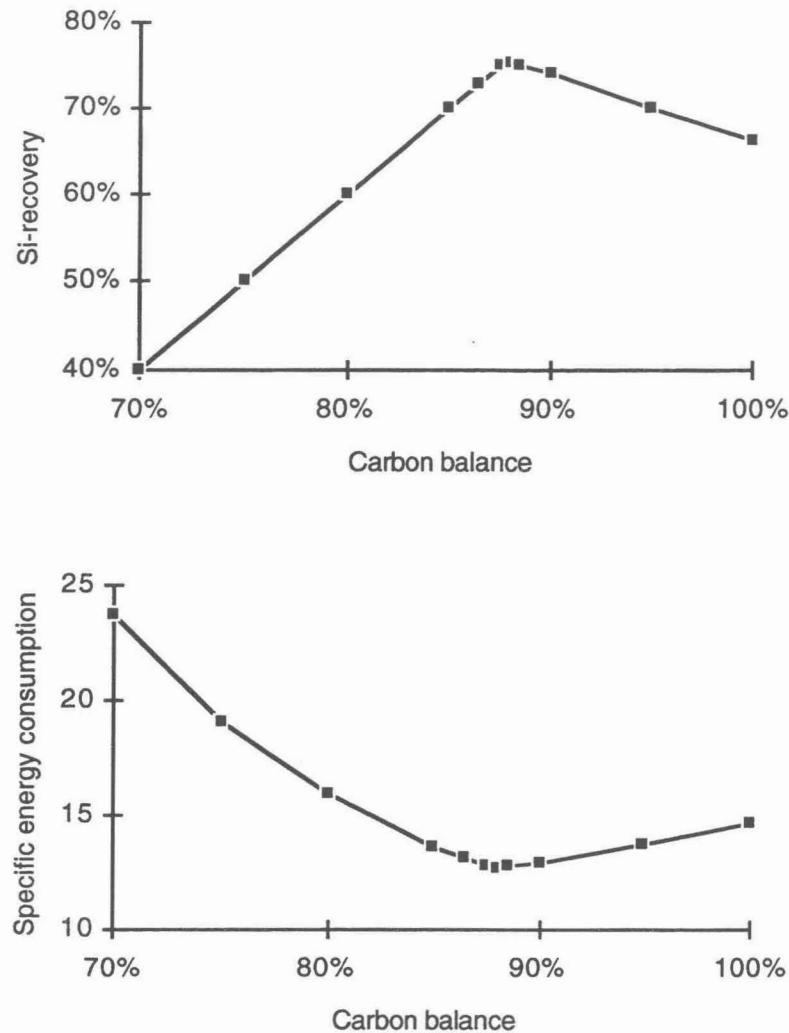


Figure 5 - Results from a typical case study (exercise) with the stoichiometric model: Silicon recovery (Si in charge recovered as tapped metal) and specific energy consumption (kWh/kg Si tapped) as function of the carbon balance in the charge. 83% efficiency has been assumed for the energy computations.

Hands-on process education

For the FeSi/Si-processes the mathematical models are lectured along with and integrated with the process chemistry. After a few lectures each participant is given a personalised floppy-disk copy of the model (Excel spreadsheet and macro sheet) along with some carefully selected exercises. The course continues with alternating computer sessions, lectures and discussions.

As a first model exercise the participants are requested to enter a given set of input data, and then perform a series of computations varying the carbon balance. For each computation the silicon recovery and the specific energy consumption are recorded. Both variables are finally plotted as function of the carbon balance^{*)}. The results are shown in figure 5. This exercise shows the fundamental result that the silicon recovery will increase by increasing the carbon balance in the charge up to an optimum value, after which the recovery decreases. Correspondingly, the specific energy consumption gets its minimum value for the same optimum carbon balance.

^{*)} 100% carbon balance is defined as the amount of carbon giving 100% Si-recovery according to the ideal (total) reaction: $\text{SiO}_2 + 2 \text{C} = \text{Si} + 2 \text{CO}$, i.e. two moles of carbon per mole SiO_2 .

While the first exercise shows the qualitative result of changing the carbon balance, the following ones deal with other parameters:

- Improved (more reactive) carbon materials are charged. The reactivity number in the model is increased. The computations show (as expected) that it is possible to run the furnace at a higher Si-recovery.
- The furnace has a segregation problem. Input values are modified by distributing carbon and quartz to the two upper chambers, one chamber being "under-coked" and the other "over-coked". The distribution of gas to the two chambers is also affected. The model calculations show how the process is negatively affected.
- Due to improper stoking procedures, the charge is partly sent directly to the hearth zone without reaction in the upper chambers. Input data is changed, and the computations show the displeasing results.
- Etc.

In principle the exercises are similar to the case studies presented in [2], but the educational value is totally different. Reading a presentation of the model, you are confronted with some theoretical presentation on what is going on in some furnace. Doing the exercises, *your* furnace is the central issue: How can you improve the silicon recovery, what are the (qualitative) effects of segregation, proper/improper stoking, etc. With such a focus along with the process of doing the exercises, the mental framework of the researchers is effectively transferred to the process metallurgists. During discussions following the model sessions, information also flows in the opposite direction, i.e. the researchers are updated on practices and ideas at the plants, including current furnace problems.

As part of the process the participants are being acquainted with some basic features of mathematical models: Simplification and limited scope of application: The stoichiometric model provides a *simplified* mental picture of the process, comprising the essential behaviour. It is, however, limited to qualitative simulations and does not capture all aspects of the process. When analysing a specific furnace problem, it should always be evaluated whether the model assumptions and the current input are relevant.

Experience and future challenges

Utilising the stoichiometric model within The Elkem University and also on more informal internal workshops, has established a common framework for process discussions within Elkem. This foundation has proved extremely valuable for transferring ideas and information between process metallurgists and researchers/theoretical experts. The model, although stationary, has even been useful for some dynamic discussions. Assume for instance that a silicon furnace is gradually accumulating SiC in the hearth region. This corresponds (among others) to diminishing the active hearth volume, implying that kinetic restrictions are slowly enhanced. Such changes can be simulated in the stoichiometric model by raising the value of the *s*-parameter, and the gradual change in process conditions can be visualised.

As a consequence of the common framework, the old saying referred in the introduction has become obsolete among Elkem's FeSi/Si-metallurgists. Consensus is no longer extraordinary.

The FeSi/Si processes are by no means fully understood. Improved understanding of various dynamic effects is, among others, requested, among Elkem's researchers as well as our process metallurgists. Presently the dynamic model is in a state where it can be used by experts only. It will, however, be evaluated whether the model (with a reasonable effort) can be transformed to an educational tool, e.g. by developing a simplified user interface. It will additionally be a challenge to design a suitable set of exercises/case studies.

For the Mn- and Cr-processes The Elkem University has clearly improved communication among the metallurgists. Contrary to the FeSi/Si-processes, there exists, however, no process model similar to the stoichiometric one, and the lack of such a common foundation is an evident drawback. Work is in progress to establish the necessary process understanding and model

framework, among others as part of a Dr.ing. (PhD) study at The Norwegian Institute of Technology [11]. Hopefully, proper model(s) will be completed in the not too distant future.

CONCLUSIONS

A comparatively simple stoichiometric model for the (ferro)silicon process has established a sound foundation for Elkem's process understanding for the FeSi/Si-processes. The model is now an integrated part of Elkem's continued education for process metallurgists.

The success of the models is probably due to the combined effect of

- Simple mental framework
- Comprising the fundamental aspects of the process
- User-friendly input/output
- Quick calculations
- Integrating the model as part of the continued education for process metallurgists

The model framework has proven valuable for exchanging theories, ideas, and experience between Elkem's research specialists and process metallurgists.

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