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SIMP

COMPUTATIONAL THERMODYNAMICS IN THE MODELLING OF IRON AND STEELMAKING PROCESSES

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In order to model iron and steelmaking processes, it is necessary to have suitable tools for the mathematical consideration of all the relevant phenomena occuring in these processes. Chemical reactions are an essential part of nearly all iron and steelmaking processes and therefore it is mandatory to know how to model the reactions when creating process models for iron and steel industry. Modelling of chemical reactions consists of two areas: *i.e.* determination of chemical equilibria (thermodynamics) and consideration of the rate phenomena (namely kinetics and transport phenomena).

Temperatures of pyrometallurgical iron and steelmaking processes are high and hence the chemical equilibria is in many cases reached relatively quickly, although there are certain phenomena in which the rate phenomena - mainly mass transfer - plays an important role also in higher temperatures. Modelling of fast reactions is relatively simple since the consideration of the rate phenomena can be neglected and mere thermodynamics give sufficiently accurate presentation of the reactions. On the other hand, thermodynamics cannot be ignored even when modelling reactions controlled by the rate phenomena. In these cases thermodynamic considerations are needed to define the driving forces for the reactions whereas the modelling of reaction kinetics and transport phenomena describes the actual rates of the considered reactions.

Within the SIMP research projects computational thermodynamics (CTD) has been used in various contexts. Both ready-made software and databases (mainly FactSage and HSC Chemistry) as well as more custom-made approaches have been used. The computational results have been verified by comparing them with the results of laboratory experiments, industrial campaigns and samples as well as values presented in the literature.

Softening and melting behaviour of the blast furnace raw materials (*i.e.* pellets and briquettes made of recycled materials) has been investigated by computing phase diagrams for multi-components systems containg FeO, SiO_2, CaO and MgO. Computational liquid phase fractions as a function of temperature have been used estimate the temperatures in which the softening of the pellets and briquettes starts.

Iljana M, Kemppainen A, Heikkinen E-P, Fabritius T, Paananen T & Mattila O. A new sophisticated method for evaluating the reduction-softening properties of iron burden materials. METEC & 2nd ESTAD 2015. 15-19.6.2015. Düsseldorf, Germany. 10 p.

Kemppainen A, Iljana M, Heikkinen E-P, Fabritius T, Ohno K-I, Maeda T, Kunitomo K, Mattila O & Paananen T. Softening behavior of iron ore pellets in the cohesive zone of a blast furnace. METEC & 2nd ESTAD 2015. 15-19.6.2015. Düsseldorf, Germany. 10 p.

Kemppainen A, Ohno K-I, Iljana M, Mattila O, Paananen T, Heikkinen E-P, Maeda T, Kunitomo K & Fabritius T. Softening behaviors of acid and olivine fluxed iron ore pellets in the cohesive zone of a blast furnace. ISIJ International. Vol 55. 2015. No10. pp. 2039-2046.

Reactions of the alkali-bearing minerals in the coke ash as well as ***mineral-associated CO_2 and H_2O emissions*** in coke oven and blast furnace conditions have been considered with CTD.

Gornostayev S, Heikkinen E-P, Heino J, Fabritius T & Härkki J. Mineral-associated CO_2 and H_2O emissions during the production of metallurgical coke. Steel research international. Vol. 84. 2013. No. 11. pp. 1104-1109.

Gornostayev S, Heikkinen E-P, Heino J & Fabritius T. Fe-Si particles on the surface of blast furnace coke. International journal of minerals, metallurgy and materials. Vol 22. 2015. No 7 pp. 697-703.

Gornostayev S, Heikkinen E-P, Heino J, Huttunen S & Fabritius T. Behavior of alkali-bearing minerals in coking and blast furnace processes. *Submitted to* Steel research international.

CTD is one ***part of the process model created to simulate the AOD process***. Created model have been used *e.g.* to evaluate the effect of different process conditions on the carbon removal efficiency and to estimate the metal and slag compositions as a function of blowing time.

Visuri V-V, Järvinen M, Sulasalmi P, Heikkinen E-P, Savolainen J & Fabritius T. A mathematical model for the reduction stage of the AOD process. Part I: Derivation of the model. ISIJ International. Vol. 53. 2013. No. 4. pp. 603-612.

Visuri V-V, Järvinen M, Savolainen J, Sulasalmi P, Heikkinen E-P & Fabritius T. A mathematical model for the reduction stage of the AOD process. Part II: Model validation and results. ISIJ International. Vol. 53. 2013. No. 4. pp. 613-621.

CTD has also been used to estimate ***the existence of different constituents in very high temperatures as a part of the development of the optical emission spectrum measurements***. These measurements have been used to characterize the process conditions in the electric arc furnace used in the stainless steelmaking.

Aula M, Leppänen A, Roininen J, Heikkinen E-P, Vallo K, Fabritius T & Huttula M. Characterization of process conditions in industrial stainless steelmaking electric arc furnace using optical emission spectrum measurements. Metallurgical and materials transactions B. Vol. 45. 2014. No. 3. pp. 839-849.

Distribution of sulphur between inclusions and molten steel has been computed as a function of Ca-content and the results have been compared with the analyses of industrial samples.

Heikkinen E-P, Alatarvas T, Määttä L, Antola T, Leinonen M, Ollila S & Fabritius T. A thermodynamic study on the distribution of sulphur between inclusions and molten steel. 9th International Conference on Clean Steel. 8-10. 9. 2015. Budapest, Hungary. OMBKE. 11 p.