

Implementation and Validation of a Three-Dimensional Multiphase-CFD-Model for Blast Furnace Processes

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In this work models capable to describe processes in the blast furnace are developed. The implementation of a CFD-model accounting for the flow of coke as well as fluids is presented. By applying separate sets of conservation equations the governing balance equations are solved for both phases. Heterogeneous reactions and heat transfer effects are modelled by implementing source terms based on correlations describing the underlying physics. This model setup has been successfully validated using a number of heat transfer problems as well as setups including heterogeneous and homogeneous chemical reactions.

1. Introduction

In the common blast furnace process, coke is used as reducing agent of iron ores to produce molten iron. This process is generally very capital and energy intensive, therefore iron and steel producing industry attempt to reduce the demands by replacing coke by alternative reducing agents such as pulverized coal, gas and other carbon carriers (Fu et al., 2011). Voestalpine Stahl GmbH in Linz (Austria) utilizes a wide variety of alternative reducing agents at blast furnace A such as oil, crude tar, natural gas and waste plastics which are injected into the raceway. However, the injection of such agents influences the processes in the blast furnace, arising the need for thorough examination of the impact on the furnace operation.

Due to the extreme conditions in blast furnaces, the application of experimental techniques to examine processes in the furnace is very limited. An alternative to such experiments is to conduct numeric simulations utilizing the methods of Computational Fluid Dynamics (CFD). In the K1-MET framework of research activities, CFD models have been developed to simulate the combined injection of waste plastic particles and heavy oil into the blast furnace raceway (Harasek et al., 2012; Jordan et al., 2010)

In the current work, an alternative method to close the material balance within the computational domain referenced as “dual grid approach” was implemented (see Figure 1). This approach accounts not only for the gas flow in the blast furnace, but also models the solid phase flow which is coupled to the gas phase.

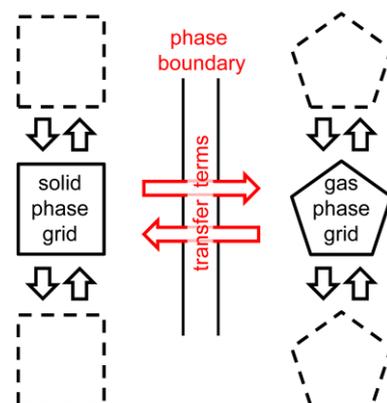


Figure 1: Scheme of coupling terms for the dual grid method.

Coupling terms for mass, species, momentum and energy are evaluated based on correlations describing the underlying physics. This provides the functionality to capture phenomena occurring within the blast furnace such as heterogeneous reactions, heat transfer and thermal conductivity effects within the coke bed, avoiding the high computational effort of a full eulerian multiphase formulation and incorporates also a simplified reaction mechanism for calculation of the high temperature conversion of the injected materials as well as the blast furnace coke.

2. CFD Model setup

The CFD solver code used for the steady state simulations is FLUENT 6.3.26, one of the leading commercially available general purpose codes with included post processing tools. FLUENT uses a finite volume discretization, for each finite control volume the physical balance equations are solved for momentum, energy, radiation, mass, turbulence quantities and species concentrations. Since some of the equations are highly nonlinear, an iterative solving procedure has to be used. Turbulence is handled by applying Reynolds averaging of the Navier-Stokes-Equations (RANS) and suitable two-equation closure formulations. An important feature of the FLUENT code is the possibility to enhance the features of the standard solver with new models by utilizing compiled user defined functions (libraries written in C programming language), which are linked dynamically to predefined solver interfaces.

In the dual-grid approach, conservation equations are solved for both, solid (e. g. coke bed) and gaseous phase. The general conservation equation of an extensive quantity in its differential form can be written as (Paschedag, 2004):

$$\underbrace{\frac{\partial \Phi}{\partial t}}_{\text{storage term}} = - \underbrace{\nabla(\mathbf{v}\Phi)}_{\text{convective term}} - \underbrace{\nabla J_{\Phi}}_{\text{molecular transport}} + \underbrace{S_{\Phi}}_{\text{source term}} \quad (1)$$

In equ. 1, Φ represents an arbitrary extensive quantity that is to be replaced by the considered quantity, e.g. species concentration ($\Phi = Y_i$) in the case of a species balance in the fluid mixture. The dual grid model was set up by implementing source terms (last term in equ. 1) in the conservation equations describing the physical processes, i.e. species mass sources due to gasification reactions or heat sources in the case of heat transfer between solid and gas phase and due to heat of heterogeneous reactions.

The implementation of the dual grid model has been validated for a number of heat transfer problems in porous media of different types in a wide range of operating conditions (stationary solid phase) as well as for heterogeneous and homogeneous chemical reactions (moving solid bed), see Table 1. The validation procedure was structured such, that different experimental setups from literature were implemented in CFD with increasing complexity of the physical processes, starting at simple heat transfer problems between gaseous and solid phases. The simulation results were compared to the measured data to analyze the model performance. Validation of the sub-models dealing i.e. with inert solid phase including heat-transfer are reported elsewhere (Maier et al., 2012), the focus of this work is laid on the discussion of the coke gasification model.

Table 1: Overview of validation cases for dual grid method

| validation case | temperature range | solid matter | solids structure | reactivity |
|---|-------------------|-----------------|------------------|------------------------------|
| closed system with respect to mass transfer gas flow: natural convection | up to 1250°C | coke pebbles | bed of spheres | inert |
| open system gas flow: forced flow through fixed bed | 20 to 100°C | ceramic pebbles | bed of spheres | inert |
| porous burner: open system | up to 1500°C | SiC | foam matrix | homogeneous |
| coke gasification | up to 1100°C | coke | coke bed | homogeneous heterogeneous |

3. Coke gasification model

In the blast furnace process, lump ore, ore sinter or ore pellets are fed as raw material for the production of pig iron. Additionally, coke is fed as fuel and as carbon-carrier. While the feed materials in the shaft furnace proceed downwards, besides direct reduction of ore, coke is also subjected to heterogeneous reactions with the hot counter-current gas flow. The coke gasification produces gas species that interact with the iron ore and contribute to ore reduction.

3.1 Intrinsic kinetics

A set of heterogeneous gasification reactions was implemented to model the coke utilization. The reaction equations and intrinsic kinetics are summarized in Table 2. The parameters in the kinetic expressions are valid for coke from wood pyrolysis, as charcoal of this type was used in the experiments that were adopted for model validation (Van de Steene et al., 2010).

Table 2: Intrinsic kinetics of heterogeneous reactions

| Equation | Kinetic expression | ν | ref. |
|--|--|-------|------|
| $\text{CH}_x\text{O}_y + (x/4 - y/2) \text{O}_2 \xrightarrow{k_{\text{O}_2}} \text{CO}_2 + x/2 \text{H}_2\text{O}$ | $k_{\text{O}_2} = 4.8 \cdot 10^9 \cdot e^{-\frac{16731}{T}} \left[\frac{\text{mol m}^{3\nu}}{\text{kg mol}_{\text{O}_2}} \right]$ | 0.59 | [1] |
| $\text{CH}_x\text{O}_y + \text{CO}_2 \xrightarrow{k_{\text{CO}_2}} 2\text{CO} + y \text{H}_2\text{O} + (x/2 - y) \text{H}_2$ | $k_{\text{CO}_2} = 7.8 \cdot 10^{10} \cdot e^{-\frac{29456}{T}} \left[\frac{\text{mol m}^{3\nu}}{\text{kg mol}_{\text{CO}_2}} \right]$ | 0.13 | [1] |
| $\text{CH}_x\text{O}_y + (1 - y) \text{H}_2\text{O} \xrightarrow{k_{\text{H}_2\text{O}}} \text{CO} + (1 + x/2 - y) \text{H}_2$ | $k_{\text{H}_2\text{O}} = 3.42 \cdot T_p \cdot e^{-\frac{15600}{T}} \left[\frac{\text{mol m}^{3\nu}}{\text{m}^2 \text{s mol}_{\text{H}_2\text{O}}} \right]$ | 1 | [2] |
| $\text{CH}_x\text{O}_y + (2 + y - x/2) \text{H}_2 \xrightarrow{k_{\text{H}_2}} \text{CH}_4 + y \text{H}_2\text{O}$ | $k_{\text{H}_2} = 0.00342 \cdot T_p \cdot e^{-\frac{15600}{T}} \left[\frac{\text{mol m}^{3\nu}}{\text{m}^2 \text{s mol}_{\text{H}_2}} \right]$ | 1 | [3] |

[1] (Rumpel, 2000), [2] (Hobbs et al., 1992), [3] (Tepper, 2005); ν =reaction order, stoichiometric coefficients $x = 0.292$, $y = 0.0085$.

In the experiments the coke was prepared by pyrolysis of wood chips at 750 °C for 1 h. Therefore, the presented gasification model does not consider the drying process, solids are assumed to be free of moisture. However, drying kinetics can be added if wet material is treated.

3.2 Boundary layer diffusion

Prior to reaction with solid coke, gaseous reactants need to be transported to the particle surface. The driving force for this mass transfer process is the concentration difference between surrounding gas phase and near the surface. This problem is formulated as boundary layer diffusion problem. In this work, multicomponent diffusion coefficients for each of the gas-phase species, D_{im} , are calculated based on the relationship of Wilke (1950) and binary diffusion coefficients D_{ij} using the correlation of Fuller et al. (1969) (v_i, v_j ... diffusion volumes of gas molecules; T_f, T_p, T_m ... fluid, particle and mean temperature; M_i, M_j ... molecular weight; p ... pressure; x ... mole fraction; N ... number of species):

$$D_{ij} = \frac{0.00143 \cdot T_m^{1.75} \cdot \sqrt{\frac{1}{M_i} + \frac{1}{M_j}}}{p \sqrt{2} (\sqrt{v_i} + \sqrt{v_j})^2} \quad D_{im} = \frac{1}{\sum_{j=1, j \neq i}^N \frac{x_j}{D_{ij}}} \quad T_m = \frac{T_f + T_p}{2} \quad (2)$$

The thickness of the boundary layer depends on the fluid dynamics and transport properties of the system and is considered by implementation of the dimensionless Sherwood-number Sh . A variety of expressions correlating Reynolds (Re) and Schmidt number (Sc) to Sh is available, accounting for different flow regimes. Here, the correlation of Petrovic et al. (1968), applicable to fixed bed conditions, is used to compute the mass transfer coefficient β (ε ... fixed bed porosity, d_p ... particle diameter):

$$Sh = \frac{\beta \cdot d_p}{D_{im}} = \frac{0.357}{\varepsilon} Re^{0.641} Sc^{1/3} \quad (3)$$

3.3 Pore diffusion

The diffusion of educts to the actual reaction sites in the pore structure of coke particles is considered by introduction of an effectiveness factor η (Liu et al., 2004). This approach allows for the estimation of

the degree of pores that is utilized in the considered heterogeneous reaction and therefore the decrease of the reaction rate due to pore diffusion:

$$\eta \triangleq \frac{\text{reaction rate accounting for diffusion}}{\text{intrinsic reaction rate}}$$

The effectiveness factor is a function of educt concentration in the particle pores and the intrinsic reaction rate and can be expressed by the Thiele-modulus Φ . For a spherical particle, η is estimated as (Liu et al., 2004):

$$\eta = \frac{1}{\Phi} \left(\frac{1}{\tanh \Phi} - \frac{1}{\Phi} \right) \quad (4)$$

with the Thiele modulus given by (Rumpel, 2000) (k ... intrinsic reaction rate, ρ_p ... coke density, C ... species concentration):

$$\Phi = \frac{d_p}{2} \sqrt{\frac{1-v}{2} \frac{k \cdot \rho_p \cdot C_{\text{educt,surface}}^{1-v}}{D_{\text{eff}}}} \quad (5)$$

where the effective diffusion coefficient D_{eff} (diffusion inside the pores) is calculated accounting for Knudsen diffusion (Gemmen et al., 2006).

3.4 Effective reaction rate

Finally, the effective reaction rate k_{eff} is calculated considering the educt diffusion through the boundary layer of a coke particle as well as pore diffusion in internal particle structures, implementing diffusion processes as "serial resistances" (a_{coke} ... specific particle surface area):

$$k_{\text{eff}} = \left(\frac{1}{\beta \cdot a_{\text{coke}} \cdot C_{\text{educt}}^{1-v}} + \frac{1}{\eta \cdot k} \right)^{-1} \quad (6)$$

Using this approach the effective reaction rate can be calculated for a wide temperature range, accounting for limitation of heterogeneous reactions by intrinsic reaction rates at lower operating temperature (zone I), limitation by pore diffusion at intermediate temperatures (zone II) and boundary layer diffusion at high temperatures (zone III). The rates for coke oxidation in the gasification mixture as applied in this work are presented in Figure 2.

The dependence of boundary layer diffusion on temperature is in the order of $T^{1.75}$ (Eq. 2), while intrinsic reaction kinetics are of order e^T (based on Arrhenius-type kinetics). As a consequence, at higher temperatures educt concentration in the coke particle declines and the limiting step of a heterogeneous reaction is posed by the diffusion of educts towards the particle surface.

4. Experimental: Validation case

The implementation of the dual grid model was validated against published experimental data comprising a fixed bed reactor for wood char gasification in continuous operation mode Van de Steene et al. (2010), see Figure 3. Continuous operation is very important if it comes to the representation of the setup in a CFD-model: by continuous operation mode, steady-state operating characteristics

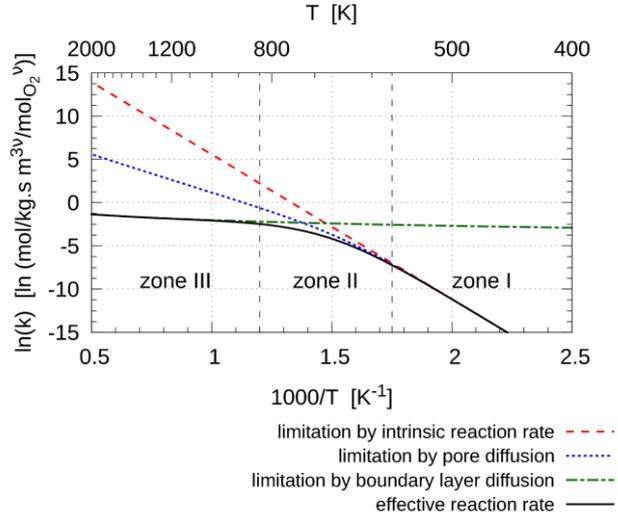


Figure 2: Rate of coke oxidation as function of temperature. Operating conditions: gas velocity $v_g=0.5$ m/s, $p=1013$ mbar, gas mixture: 30%(v/v) H_2O , 8%(v/v) CO_2 , 2.7%(v/v) O_2 , 59.3%(v/v) N_2 .

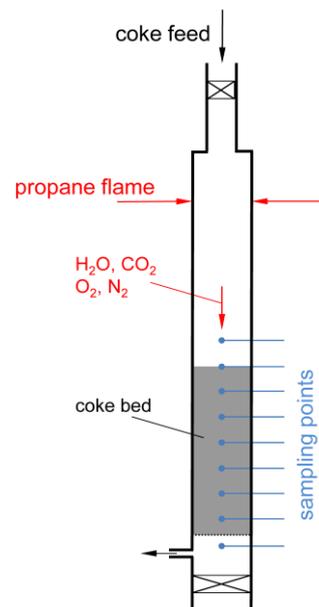


Figure 3: Sketch of the continuous fixed-bed reactor used in the work of Van de Steene et al. (2010).

are achieved and thus it is not necessary to apply time-discretization of the conservation equations, drastically reducing the computational demand.

The experimental reactor is fed with coke particles from top (feed rate 28 g/min, ultimate analysis: 89.8%(w/w) C, 2.2%(w/w) H, 6.1%(w/w) O, 0.1%(w/w) N). The reacting gas was produced by propane flames located above the coke bed (gas conditions prior to coke bed: 1020 °C, 30%(v/v) H₂O, 8%(v/v) CO₂, 2.7%(v/v) O₂, 59.3%(v/v) N₂, flow rate 226 L_{STP}/min). Instrumentation included sampling and measuring probes in 10 cm intervals along the fixed bed, allowing for determination of temperature and species concentration profiles in the reactor (Van de Steene et al., 2010).

5. Simulation results

The left diagram in Figure 4 shows the calculated profiles of coke consumption due to heterogeneous reactions. Near the surface of the coke bed, steep gradients are found due to the onset of coke oxidation. This reaction is strongly exothermic and therefore delivers heat as well as additional gasification agents for the gasification reactions including CO₂ and H₂O as educts. The latter reactions also contribute to the release of H₂ that is subsequently consumed by the methanation reaction, however, at comparatively low reaction rates (according to the low a frequency factors in these reactions, see Table 1). The released gaseous reaction products are also subjected to the homogeneous reaction mechanism (6 Arrhenius-type reactions).

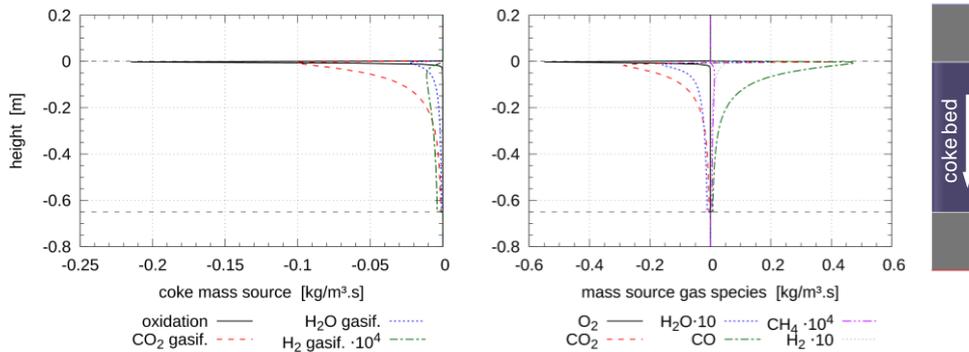


Figure 4: Simulation results: Source terms due to heterogeneous reactions.

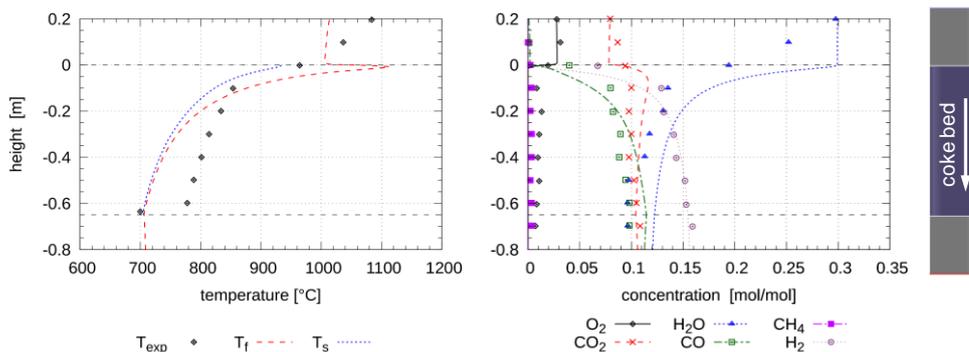


Figure 5: Temperature and concentration profiles; points: experimental data; lines: simulation results.

The trend of O₂ concentration in the gas-phase reproduces the above mentioned occurrence of the combustion reaction as the content of oxygen rapidly drops (see Figure 5), also a distinct peak in gas-phase temperature is predicted. Further downstream heat is consumed by endothermic gasification reactions.

Most important for the blast furnace process is the CO₂-gasification of coke (Boudouard reaction) due to the formation of CO, desired for the ore reduction process. The concentrations of CO as well as H₂ rapidly increase in the upper region of the bed. In accordance to experiments it was found that this is the most reactive zone, as approx. 80 % of the final values of the species concentrations are reached after 10 cm.

6. Summary and Conclusions

A model describing the two-phase flow of fixed coke beds under gasification conditions was implemented and validated. The comparison of simulation results to reference data from literature showed good agreement. In the next step the model setup will be applied to the real blast-furnace geometry. The model predictions will be used for the optimization of operating conditions of the blast furnace to contribute to a further decrease of the environmental impact of such facilities, also aiming at further improvement of plant efficiency and economics.

Acknowledgements

The presented work has been funded by K1-MET and FFG Forschungsförderungsgesellschaft, Austria.

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