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A Coupled CFD-DEM Approach to Model Reactive Granular Beds

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Abstract: Packed and moving bed reactors are widely used in process industry to process granular material. Shaft furnaces are one example of this. Due to their counterflow layout, a high thermal efficiency can be achieved. Shaft furnaces have a wide range of length and time scales that makes them challenging to model. Geometric details, like injection nozzles, are smaller than the particle size, which need a computationally highly expensive resolved Discrete Element Method (DEM) approach. To overcome this problem, a computing technique called Volume Fraction Smoother (VFS) was developed. Since the time scales in those systems reach from milliseconds for the particle collisions to hours of process time, the process time scale must be separated to model a quasi-steady state with reasonable computing time. For this, the Time Scale Splitting Method (TSSM) was introduced. This method was also adapted to model the self-heating behaviour of direct reduced iron (DRI).

Keywords: CFD-DEM coupling, Time scale splitting method, Volume fraction smoother, Packed bed, Moving bed

Ein gekoppelter CFD-DEM-Ansatz zur Modellierung reaktiver Schüttungen

Zusammenfassung: Schüttschichtreaktoren werden in der Thermoprozesstechnik in verschiedenen Bereichen angewendet, Hierbei stellt der Schachtofen den dominanten Analgentyp da. Aufgrund seines Gegenstromprinzips ermöglicht dieser eine energieeffiziente Wärmebehandlung. Schachtöfen weisen eine große Bandbreite an Längen- und Zeitskalen auf, was deren Modellierung sehr rechenintensiv gestaltet, so dass die Modelle oft nicht auf industrielle Fragestellungen angewendet werden können. Es ist notwendig, kleine geometrische Details, wie beispielsweise die Brennerdüsen, im Rechennetz aufzulösen. Da hierbei jedoch Zellen, die kleiner als die Partikel sind, entstehen, wären diese im Rechengitter aufzulösen, was sehr rechenintensiv ist. Um dieses Problem zu lösen, wurde eine Rechentechnik namens Volume Fraction Smoother (VFS) entwickelt. Die Zeitskalen bei einer bewegten reaktiven Schüttung bewegen sich von Millisekunden für die Partikelkollisionen bis zu Stunden Prozesszeit. Damit das Modell numerisch effizient gestaltet werden kann, ist eine Trennung dieser Zeitskalen notwendig, um einen quasistationären Zustand zu beschreiben. Zu diesem Zweck wurde die Time Scale Splitting Method (TSSM) entwickelt. Eine modifizierte Variante dieses Modell kann auch zur Beschreibung des Selbsterwärmungsverhaltens von Schüttungen verwendet werden, im konkreten Fall wird die Selbsterwärmung durch Reoxidation von direkt reduziertem Eisen (DRI) angeführt.

Schlüsselwörter: CFD-DEM-Kopplung, Time-Scale-Splitting-Methode, Volume fraction smoother, Reaktive Schüttung

1. Introduction

The presented model was initially developed for shaft furnaces. These are used in different industries for raw material production. The most common use is the production of burned lime. Also, raw materials for refractory production are processed in shaft furnaces. Approximately 90% of the worldwide production of direct reduced iron (DRI) is accomplished by the MIDREX and HYL-ENERGIRON processes [1]. Both represent gas-fired shaft furnaces. Since shaft furnaces are used in such a wide range of industries, it is important to model and analyze those processes to improve and adapt them. To model a shaft furnace, the gas and granular phases must be solved coupled. An Eulerian approach for the granular phase is computationally

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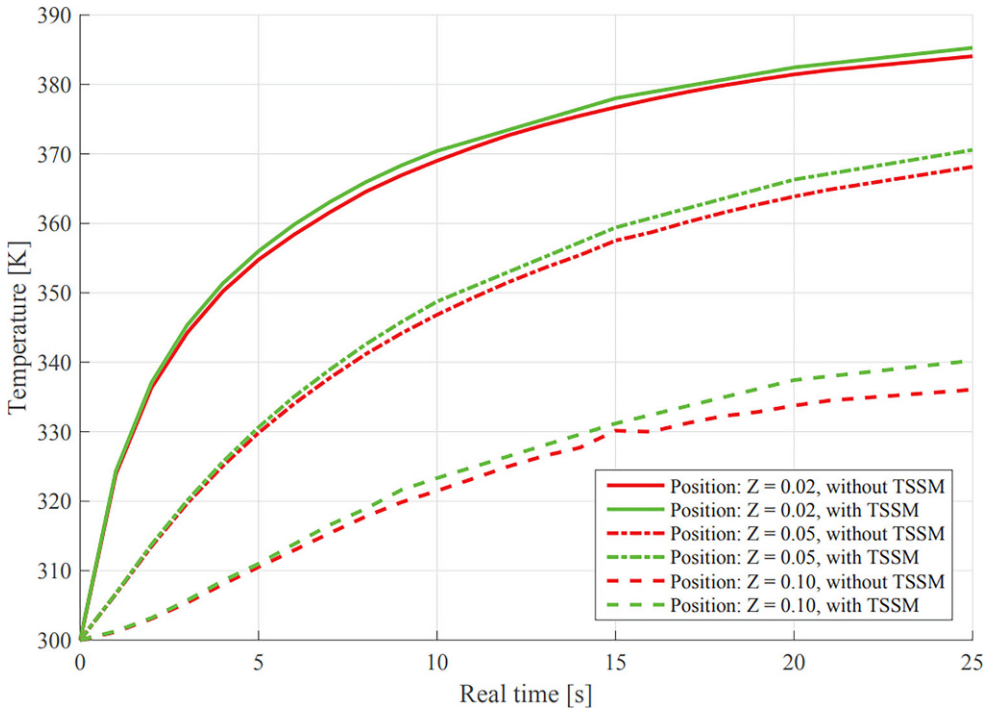

Fig. 1: Transient temperature profile in different heights for the heat up of a packed bed of ten 10 mm particles. The *red curves* represent the original case. For the *green curves*, the TSSM with an acceleration factor of 200 was used [2]

efficient but also numerically diffusive and cannot resolve certain flow characteristics of the granular phase. Therefore the Discrete Element Method (DEM) approach was chosen. Till a non-resolved DEM approach cannot be used in certain shaft furnaces due to small geometrical details, smaller than the particle size, and a resolved DEM approach is numerically too costly, an intermediate method needs to be developed. This method is called Volume Fraction Smoother (VFS), where the particles are represented over several gas phase cells without a change to the Computational Fluid Dynamics (CFD) grid. To reduce the calculation time of the system until a quasi-steady state condition is achieved, the time scales between the granular phase and the gas phase are separated by the Time Scale Splitting Method (TSSM) [2]. This method was also used to model the self-heating behaviour of DRI.

2. Model Description

The model is based on OpenFOAM [3], where implementations for versions 2.4 and 6 are developed. The model can be separated into the CFD part, which describes the fluid phase and homogeneous reactions, and the lagrangian DEM part, which models the granular phase.

2.1 Time Scale Splitting Method (TSSM)

This method uses two different timesteps: The original timestep is used for computing the gas phase equations and forms the basis for the collision sub-cycles for the DEM particles. The accelerated timestep is used for the fluxes on the DEM side, like heat, species, and mass fluxes of the particles. These two timesteps are linked by a pre-defined acceleration factor. Because the fluxes between the phases are corrected with the acceleration factor, the conservation of mass, energy, and species is fulfilled. Pollhammer [2] evaluated the TSSM by modelling the transient heat-up of a packed bed containing ten particles with a diameter of 10 mm. These particles have an initial temperature of 300 K and were heated up by air with a superficial velocity of 0.5 m/s and a temperature of 400 K by convection from the bottom. Here an acceleration factor of 200 was used. Figure 1 shows the comparison between the TSSM and a non-accelerated heat-up of the packed bed for different heights. The largest deviation could be observed for the top particle at a height of 100 mm. Here the deviation of the temperature is 8% for this fully-phase-coupled transient case. The calculation time could be reduced by 98% for this evaluation case.

2.2 Fluid Phase

2.2.1 Volume Fraction Smoother (VFS)

Due to geometrical details in certain sections in the computing grid, it is possible that a particle there is larger than the computing cell, which would lead to an unphysical volume fraction greater than one on the granular phase and a negative volume fraction on the gas phase. Here the volume fraction must be distributed over several cells. The penalisation method [4] addresses this issue but is quite expensive in terms of computing resources. Gauss equation filters are fast but generate a volume fraction gradient over several cells. To address this issue, Pollhammer [2] developed an iteration algorithm called VFS. For the volume fraction, a threshold value is defined. If the volume fraction is higher than this threshold value, the volume fraction is

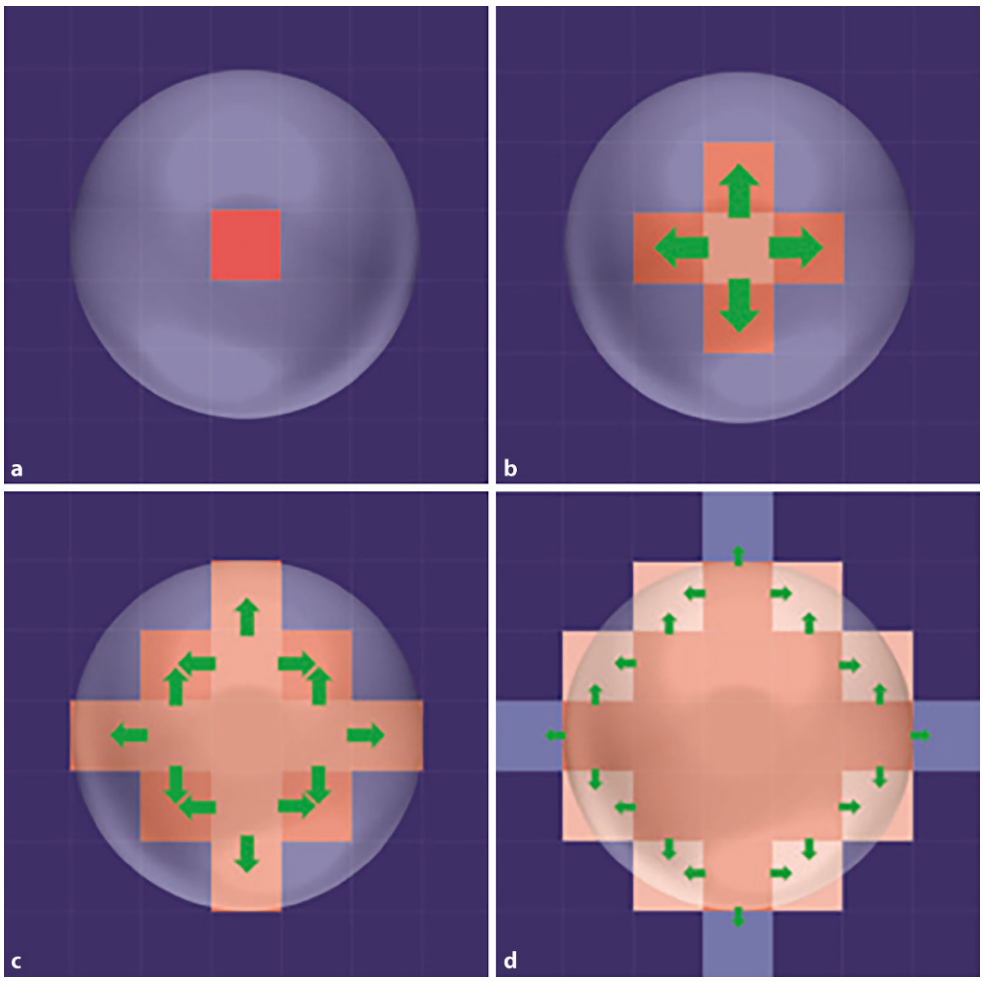

Fig. 2: Graphical explanation of the Volume Fraction Smoother. The volume fraction is shifted to neighbouring cells till the volume fraction is lower than a set threshold value. **a** Initial volume fraction, **b** First smoothing iteration, **c** Section smoothing iteration, **d** Final smoothing iteration [2]

shifted to the neighbour cells. Due to this shift the volume fractions of these cells are higher than the threshold value (Fig. 2b). During this process the volume fraction is conserved. This process is repeated (Fig. 2b, c) till all cells are below the threshold value.

2.2.2 Flow

The furnace model predicts the flow through the granular bed, as well as the free fluid flow outside the bed. The momentum equation (Eq. 1) can be formulated for both regimes. Here ρ is the gas phase density, ε the gas phase volume fraction, $\vec{u}$ the velocity vector of the gas phase, p the pressure, and $\vec{g}$ the gravity vector.

$$\frac{\partial(\rho\epsilon\vec{u})}{\partial t} + \vec{u}\nabla(\rho\epsilon\vec{u}) + S_\mu = -\nabla(p\epsilon) + \rho\epsilon\vec{g} \tag{1}$$

The source term S_μ for the viscous forces must be formulated differently inside and outside of the granular bed. If the granular phase's volume fraction is larger than 0.1, a granular bed is assumed, and the Ergun equation (Eq. 2; [6]) is used. Here η is the dynamic viscosity, $\underline{d_p}$ the average particle diameter, and $\overrightarrow{u_{rel}}$ the relative velocity vector between the phases. For slow-moving beds, the relative velocity can also be replaced by $\vec{u}$, the velocity vector of the gas phase.

$$S_\mu = \left[150\frac{(1-\epsilon)^2}{\epsilon^3}\frac{\eta\overrightarrow{u_{rel}}}{\underline{d_p}^2} + 1.75\frac{(1-\epsilon)}{\epsilon^3}\frac{\eta\overrightarrow{u_{rel}}\left|\overrightarrow{uu_{rel}}\right|}{\underline{d_p}}\right]\frac{1}{\epsilon(1-\epsilon)} \tag{2}$$

Outside of the granular bed, the source term S_t is modelled for a free turbulent flow (Eq. 3). Here the effective viscosity μ_{eff}, representing the sum of the molecular and turbulent viscosity, is modelled by a Reynolds-Averaged Navier-Stokes approach, like the k-ε turbulence model [5]. To model laminar flow, the turbulent viscosity can also be set to zero.

$$S_\mu = \mu_{eff}\nabla^2(\epsilon\vec{u}) + \frac{1}{3}\mu_{eff}\nabla(\nabla\epsilon\vec{u}) \tag{3}$$

The flow formulation, including the VFS, was evaluated by Pollhammer [2] using a randomly packed bed of 14 mm glass spheres with a height of 145 mm followed by a 155 mm free flow region. As reference in-house measurements, a resolved CFD-DEM model of the same bed and the Ergun equation [6] was used. As shown in Fig. 3, the resolved DEM approach and the presented model predict nearly the same pressure drop as function of the superficial

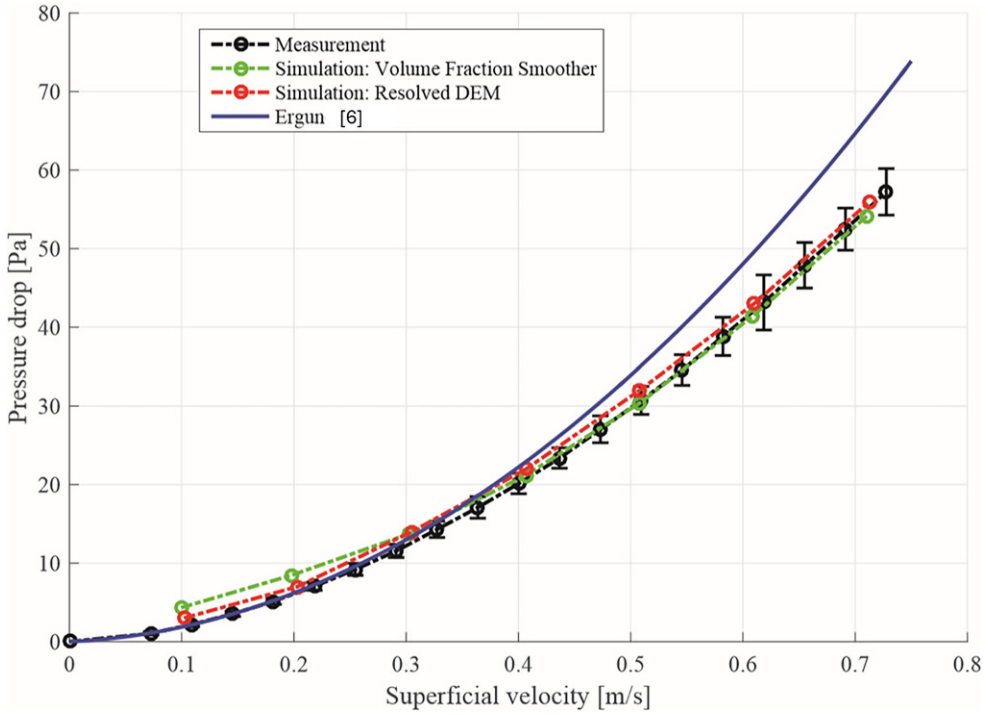

Fig. 3: Comparison of the pressure drop as function of the superficial velocity for the presented model, a resolved CFD-DEM approach, and the analytical Ergun equation [6] by Pollhammer [2]

velocity. These values are also in agreement with the measurements. The analytical Ergun equation [6] overpredicts the pressure drop.

2.2.3 Enthalpy

To obtain the temperatures in the system, an energy equation (Eq. 4) in enthalpy form is solved. Here besides the transient term, the convective transport of the enthalpy h, as well as the heat conduction are solved. The thermal conductivity is modelled by the temperature-dependent viscosity η and the Prantl number Pt. The source term for the heat transfer between the phases $S_{konv,g}$ is modelled by the approach of Gunn [7]. The source term for the heat of reaction $S_{r,g}$ is computed by the reactive thermophysical model of OpenFOAM [3].

$$\frac{\partial(\rho\epsilon h)}{\partial t} + \vec{u}\nabla(\rho\epsilon h) - \nabla\left(\frac{\eta}{Pt}\epsilon\nabla h\right) = S_{\text{konv},g} + S_{r,g} \tag{4}$$

2.2.4 Species and Reactions

The species equation (Eq. 5) has a similar form as the enthalpy equation (Eq. 5). Here, the convective transport and the diffusion of the mass fraction of a species i Y_i are solved transiently. The diffusion is modelled by the temperature-dependent viscosity η and the Schmidt number Sc. The source term $S_{p,Yi}$ describes the mass transfer to the granular phase, where heterogeneous reactions are modelled. For the source term $S_{r,g}$, for the homogeneous reactions, the Partially Stirred Reactor model (PaSR) [8], implemented in OpenFOAM [3] is used.

$$\frac{\partial(\rho\epsilon Y_i)}{\partial t} + \vec{u}\nabla(\rho\epsilon Y_i) - \nabla\left(\frac{\eta}{Sc}\epsilon\nabla Y_i\right) = S_{p,Yi} + S_{g,Yi} \tag{5}$$

2.3 Granular Phase

2.3.1 Particle Movement

The particle movements and collisions are based on the "basicKinematicCollidingCloud" implemented in OpenFOAM [3]. To model the particle contact forces, the Pair–Spring–Slider–Dashpot Model by Cundall and Strack [9] was used. The fluid forces on the particles are modelled by the Ergun–Wen–Yu–Drag model implemented in OpenFOAM [3]. For packed beds, there is also the option to freeze the particle positions.

2.3.2 Thermal Particle Model

The energy equation for each particle (Eq. 5) is formulated for the particle temperature T_p. The transient change of the particle temperature is modelled by the particle mass m_p and the temperature-dependent heat capacity of the particle $c_{p,p}(T_p)$.

$$\frac{\partial T_p}{\partial t} m_p c_{p,p}(T_p) = S_{r,p} + S_{\text{kond},pp} + S_{\text{kond},pw} + S_{\text{konv},p} + S_{\text{rad},pp} + S_{\text{rad},pw}. \tag{5}$$

To model the heat for the heterogeneous reactions and inner particle reactions $S_{r,p}$, the sum of the heat of reactions is calculated (Eq. 6), where for each temperature-dependent

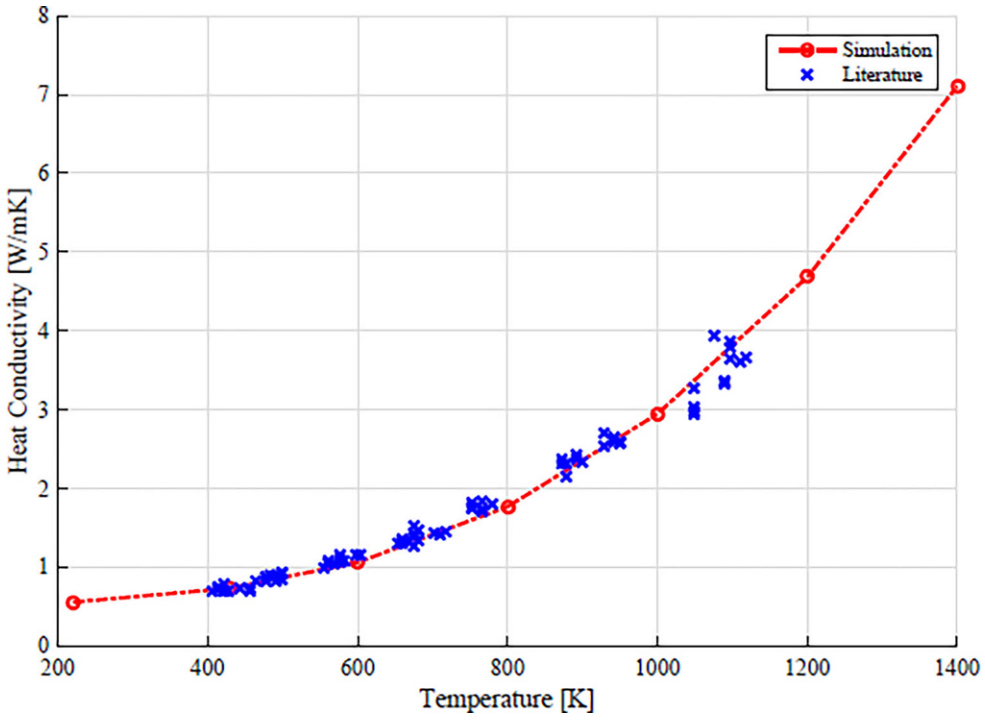

Fig. 4: Comparison of the thermal model to the measurements by Yagi and Kunii [12] by Pollhammer [2]

reaction j $h^T_{r,j}$ is calculated and multiplied by the reaction rate for the reaction rr_j.

$$S_{r,p} = \sum rr_j h^T_{r,j}. \tag{6}$$

The model also takes particle-particle and particle-wall heat conduction into account. Here the approach of Zhang [10] is used. Based on the particle forces, a contact area—A_{pp} for particle-particle contact and A_{pw} for particle-wall contact—is calculated. With the thermal resistance coefficients R_{th} and the temperature difference, the heat fluxes that represent the source terms $S_{\text{kond},pp,i}$ for particle-particle heat conduction and $S_{\text{kond},pw,i}$ for particle-wall heat conduction can be calculated (Eqs. 7 and 8).

$$S_{\text{kond},pp} = \frac{-A_{pp}}{R_{th}} \left(T_{p,i} - T_{p,j} \right) \tag{7}$$

$$S_{\text{kond},pw} = \frac{-A_{pw}}{R_{th}} \left(T_{p,i} - T_w \right) \tag{8}$$

For modelling the convective heat transfer to the gas phase $S_{konv,p}$, the model of Gunn [7] is used. Feng and Han [11] investigated these view factors for radiation in a randomly packed bed, including shading up to three particle diameters. Based on their studies, the view factors $F_{p,p}$ for particle-particle radiation and $F_{p,w}$ for particle-wall radiation can be described as a function of the particle diameter. To model the source terms for particle-particle radiation $S_{rad,pp}$ and particle-wall radiation $S_{rad,pw}$ the equation for a black body is used, where σ is the Stefan-Bolzmann constant (Eqs. 9 and 10).

$$S_{\text{rad},pp} = -\sigma F_{p,p} \left({T_{p,i}}^4 - {T_{p,j}}^4 \right) \tag{9}$$

$$S_{\text{rad},pw} = -\sigma F_{pw} \left({T_{p,i}}^4 - {T_w}^4 \right) \tag{10}$$

The thermal model, excluding reactions and convective heat transfer, was evaluated by Pollhammer [2] using the measurements of the combined heat transfer in a packed bed of 11 iron spheres by Yagi and Kunii [12]. As shown in Fig. 4, the model can predict the measured results from the lowest temperature measurement at 400 K to the highest temperature measurement at 1100 K.

2.3.3 Particle Reaction Model

Heterogeneous reactions and inner-particle reactions are handled the same way in the model. The difference is that inner-particle reactions have no source term to the gas phase. Based on the individual case, a combined reaction rate rr_j that includes the reaction kinetics and transport effects like the boundary layer or inner particle diffusion effects is modelled for a lead substance j. To describe the change of the mass fraction for a species i (Eq. 11), the lead substance must be corrected by the molar masses M_i, M_j, and the stochiometric factors v_i, v_j. The source terms for the gas phase $S_{g,Yi}$ are computed identically.

$$\frac{\partial Y_{i,p}}{\partial t} m_p = rr_i = rr_j \frac{M_i v_i}{M_j v_j}. \tag{11}$$

The change in the particle mass $m_p$is modelled by the sum of the heterogeneous reaction rates $rr_{i,g}$ (Eq. 12).

$$\frac{\partial m_p}{\partial t} = \sum rr_{i,g} \tag{12}$$

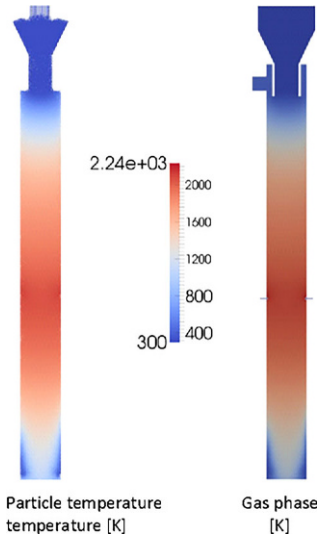

Fig. 5: Particle and gas phase temperature of the shaft furnace [13]

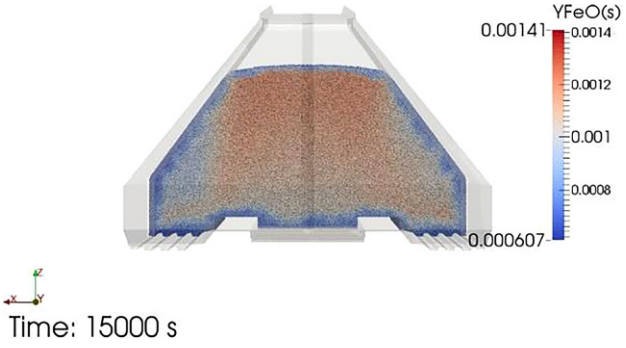

Fig. 6: Particle temperature caused by reoxidation of DRI after 15,000 s. The initial temperature was set to 333 K and the ambient temperature to 303 K

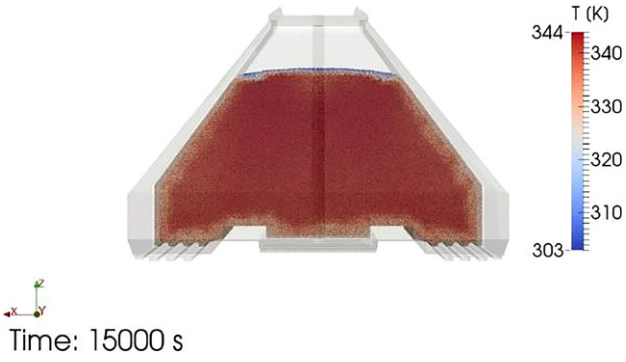

Fig. 7: Mass fraction of iron oxides in the particles due to the reoxidation

3. Application Examples

3.1 Shaft Furnace

The model of the shaft furnace consists of approximately 1.8 mio. non-reactive DEM particles range from 16 mm to 19.5 mm and 6.3 mio. hexahedral CFD cells. The furnace is heated by 12 premixed natural gas burners. For modelling the gas phase combustion, the 4-step global mechanism by Jones and Lindstedt [13] is used. The particles enter the furnace at the top and are heated up by the off-gas till they reach the combustion zone. There the temperatures reach 2243 K in the gas phase and 2209 K for the DEM particles. Then the particles are cooled by the secondary air entering from the bottom, which is consequently heated by the particles. The furnace, as can be seen in Fig. 5, was computed using the VFS and an acceleration factor of 678 for the TSSM.

3.2 Self-heating of DRI

Direct reduced iron (DRI) tends to reoxidation. This exothermic reaction leads to self-heating and can cause a thermal runaway. To investigate this behaviour, the presented model was used. Here the particle positions were frozen after filling the transport container. Since no movements in the granular phase have to be solved, it is not necessary to apply the TSSM. The heterogeneous reaction model is based on lab measurements in the differential loop reactor and is based on the temperature, the mass fraction of oxidised iron, and the oxygen concentration in the gas phase. The flow, based on natural convection, was modelled in a laminar way. Figure 6 shows the heat-up due to the reoxidation of the particles from a starting temperature of 333 K in 15,000 s. Particles near the wall are cooled mainly by particle-wall and particle-particle heat conduction from the ambient temperature of 303 K. The top layer of particles is mainly cooled by convection. The oxidation of the particles is shown in Fig. 7. Here the mass fraction of FeO is representative for different iron oxides. The oxidation is mainly driven by the available oxygen and the temperature.

4. Conclusions and Outlook

The presented coupled CFD-DEM model focuses on thermal modelling and respective reactions in granular beds. This makes the model suitable for a wide range of industrial processes. The sub-models for the heat transfer mechanisms and the flow resistance are evaluated. To model large industrial systems, numerical efficient models are needed. Here the TSSM offers a significant reduction for the transiently calculated time to the process time. The freezing of the particles is even more efficient, but this method only works for fixed beds, i.e., where no movement of particles occurs. Another method to increase numerical efficiency is coarse-grained modelling. To use coarse-grained modelling, the sub-models must be adapted correspondingly. This approach is planned for future analyses. One weak point of the model is that it is based only on spherical particles. The current approaches and sub-models would also work for a multi-sphere approach. Accounting for complex particle shapes is another model improvement for the future.

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Conflict of interest. C. Spijker and W. Pollhammer declare that they have no competing interests.

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