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Numerical investigation on particle swelling in spray roasting reactors

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ABSTRACT

Spray roasting of metal chloride solutions is frequently used in steel industries to recover pickling liquids. As spray roasting reactors are difficult to characterize experimentally, computational fluid dynamics simulations have been used to investigate reactor performance. These simulations require a particle formation model, which describes the particles size history including the characteristic effect of particle swelling. Based on available literature, different swelling models are compared by simulations of an industrial scale reactor. The influence of particle swelling is discussed. The results clearly indicate the necessity to investigate particle swelling, potential collision effects and fragmentation for sound simulation of spray roasting reactors.

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1. Introduction

Spray roasting reactors are useful tools to convert metal chloride or metal sulphide solutions to metal oxides and recover the chlorine or sulphur content (Peek, 1996). An example is the regeneration of iron chloride solutions in steel industries. Steel surfaces are pickled with aqueous hydrogen chloride to remove oxide layers from the surface. During this process, HCl is consumed forming $FeCl_2$ and small amounts of $FeCl_3$ in the solution, which leads to reduced pickling ability. Instead of dumping the spent pickling liquid, thermal regeneration is a feasible technique to recycle HCl and to produce iron oxides as valuable by-product (Kladnig, 2003).

The global chemical reaction in this process is

$$4FeCl_2 + 4H_2O + O_2 \rightarrow 2Fe_2O_3 + 8HCl - 55,0\ kJ/mol_{Fe} \quad (1)$$

Although the reaction is slightly exothermal, the typical water content of about $70\%_{mass}$ of water in the solution requires additional heat input, which is typically provided by natural gas combustion. To improve the process efficiency and to shorten evaporation and chemical conversion times, the solution is sprayed into the reactor, forming solid iron oxide particles from the solution.

The sprayed droplets undergo a multi-step conversion process in the spray roasting reactor (Beck et al., 2007b). The process starts with the evaporation of water ($T = 373$ K). During this process, the iron chloride concentration increases at the droplet surface, until the surface becomes impermeable for water vapor, causing increasing pressure which leads to swelling of the particle, producing particles with a diameter larger than the initial droplet diameter. When all water has been evaporated (note, that due to the tendency of iron chloride to form hydrates, part of the water evaporates at temperatures up to 538 K), the chemical conversion process starts.

Typical industrial scale spray roasting reactors are relatively large (more than 10 m high and 5 m in diameter) and work at high operating temperatures (~1000 K) (Beck et al., 2007b; Johansson et al., 2010; Schiemann et al., 2013; Westerberg et al., 2011). Additionally, the atmosphere inside these reactors contains large fractions of HCl, the flow field is turbulent and the droplet size distribution of the sprayed HCl solution is relatively wide (Beck et al., 2007b; Schiemann et al., 2015, 2013). These conditions render a detailed experimental analysis in industrial scale reactors difficult when the characterization of the iron oxide particles is of interest. Measurements which address the gas phase properties are possible under these turbulent conditions, e.g. gas temperature profiles as presented in Johansson et al. (2010). Additionally, the plant roasting performance by detailed analysis of iron oxide samples produced under different operational parameters extracted at the particle outlet has been determined experimentally (Ferreira and Mansur, 2011). For deeper insight, numerical studies, namely computational fluid dynamics (CFD) simulations were used to investigate the effect of geometric variations in reactor design (Johansson et al., 2014; Westerberg et al., 2011).

When the particle formation and reaction process is of deeper interest, lab-scale experiments become important. Beck et al. investigated the formation of iron oxide particles in a small scale reactor with mono-disperse droplets (Beck et al., 2007a) in the diameter range of 100 μm, which led to a numerical particle formation

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model used in CFD simulations of a large scale reactor (Beck et al., 2007b). This model was expanded by Schiemann et al., who also carried out experimental work on 100 μm droplets (Schiemann et al., 2012) to augment the insight into the particle formation process. Their model was the first to include particle swelling, which leads to the characteristic formation of particles shaped as hollow spheres. This model was used for CFD simulations of industrial scale spray roasters (Schiemann et al., 2013).

As the previous experimental work focused on particles in the size range of 100 μm (Beck et al., 2007a; Schiemann et al., 2012), but the prevailing particle size distribution in iron chloride spray roasting extends from a few μm to nearly 1 mm (Schiemann et al., 2013), a new experimental approach was used to investigate the particle formation process for droplets in the upper size limit. The experiments for the investigation of smaller particles were carried out using drop tube reactors with falling droplets/particles, but the drying time for droplets at the upper size limit exceeds the residence time in drop tube reactors. Therefore, droplets of approx. 1 mm diameter were dried by laser heating in an acoustic levitator (Schiemann et al., 2015). These experiments added information on the formation of cenospheres from larger droplets of iron chloride solution. It was shown, that the particle diameter decreased in these experiments, but was still larger than a resulting solid spherical particle would have been, indicating minor but still relevant swelling.

Based on the experimental findings in (Schiemann et al., 2015, 2012), this paper evaluates the influence of particle swelling modelling on CFD simulations of a typical spray roaster. Three different mathematical models to fit the droplet/particle diameter correlation are used to compare the influence of different assumptions for particle swelling. As the results show, current literature data provide a fundamental base for reactor modelling, but the sensitivity of reactor simulations on particle swelling demands to handle this effect with care.

2. Set-up

A generic geometry of a typical industrial iron chloride spray roaster has been developed according to Johansson et al. (2014), a quarter section of the reactor is depicted in Fig. 1. The total height of the considered domain is 20 m with a diameter of 9 m. The diameters of gas and particle outlet are 1.4 m and 1 m respectively. The burner, which is only partially simulated to keep the gas combustion model simple for acceptable computation times, has a diameter of 0.3 m. The computational domain was limited to one quarter of the total reactor using a symmetric design to reduce the computational effort. Of course, using symmetry conditions can have measurable effects on calculated flow field, but compared to results of previous simulations of spray roasters (Beck et al., 2007b; Schiemann et al., 2013) without symmetric boundary conditions no significant differences were found, which justifies the approach. A hexagonal mesh with 220,000 cells was used, and mesh dependency effects were found to be negligible for the questions which are investigated in the current work.

The energy demand of the process is in the order of 2.9 $MJ/l_{solution}$ and slightly varies with plant size and $FeCl_2$ concentration in the liquid feed (Jedlicka, 1978). The natural gas feed was substituted by a partially reacted methane–air mixture with mass flow, composition and temperature given in Table 1, as the complete simulation of the burner tube requires very high computational effort and is not the major purpose of this work. The conditions (mass flow, temperature) were chosen based on the energy demand and the fact that the gas typically reacts partially in the burner tube, but complete reaction should take place in the reactor chamber, as the brick lining at the burner entrance to the reactor is limited to temperatures of 1300 K_{max}. The iron chloride solution

Table 1
Burner feed parameters, composition given in kg/kg_{total}.

$\dot{m}$ [kg/s]	0.6
T [K]	1085
CH_4	0.0184
O_2	0.1612
CO_2	0.050
H_2O	0.040

was injected at a height of 14.5 m and a radial distance of 1.7 m from the centre axis. 0.4 $kg_{solution}/s$ with an $FeCl_2$ concentration of 30% $_w$ of iron chloride were injected with a particle size distribution $Y = 1 - \exp(-d/300)^{2.48}$ (Schiemann et al., 2013), where Y denotes the cumulative particle mass below d, which is the particle diameter in μm. The nozzles (typically around 10–15 placed on a circular holder) were not resolved in the simulation. However, the injection of 1600 particles was simulated, subdivided into 20 size fractions in the range 100–450 μm, as solid cone with an initial $v_{droplet} = 10$ m/s and a cone angle of 45° directed downwards. The injections were spread over a surface of 20 cm diameter to approximate the effect of the nozzle holder.

3. Modeling approach

The simulations were carried out using the commercial CFD code Ansys Fluent 15. The general proceeding is similar to the work described in Schiemann et al. (2013, 2012), so only a brief description is given here.

An incompressible flow was simulated using the Reynolds averaged Navier–Stokes (RANS) approach, solving the continuity and momentum equations in Reynolds-averaged simulations:

$$\frac{\partial}{\partial x_i}(\overline{\rho u_i}) = 0 \tag{2}$$

$$\frac{\partial}{\partial x_i}\left(\overline{\rho u_i u_j}\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \bar{u}_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right). \tag{3}$$

where ρ denotes the gas density in a cell, t and x denote time and spatial direction (indices mark single components) and u is the velocity. μ is the turbulent viscosity. The simulations were carried out using second order upwind discretisation and pressure–velocity coupling using the SIMPLE scheme, while the PRESTO! mechanism was used for pressure.

Turbulence modelling was carried out using the k-ω-SST model (Menter, 1994), which was found to provide the best ability to consider the wall effects in the rotating gas flow typical for spray roasters (Schiemann et al., 2013). It is represented by the governing equations for the turbulent kinetic energy k and the specific dissipation rate ω:

$$\frac{\partial}{\partial x_i}(\rho k \bar{u}_i) = \frac{\partial}{\partial x_j}\left(\Gamma_k \frac{\partial k}{\partial x_j}\right) + \tilde{G}_k - Y_k + S_k \tag{4}$$

$$\frac{\partial}{\partial x_i}(\rho \omega \bar{u}_i) = \frac{\partial}{\partial x_j}\left(\Gamma_\omega \frac{\partial \omega}{\partial x_j}\right) + G_\omega - Y_\omega + D_\omega + S_\omega. \tag{5}$$

Note, that $\tilde{G}_k$represents the generation of turbulent kinetic energy by mean velocity gradients. G_ω denotes the generation of ω, and the effective diffusivity and dissipation of k and ω are given by Γ and Y, respectively. User-defined source terms are included by $S_{k/\omega}$. By default, the k-ω-SST model as implemented in FLUENT uses enhanced wall treatment, which reduces the sensitivity to y^+ thus that $y^+ < 300$ becomes acceptable.

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