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Characteristics of Flow and Temperature Distribution in a Ruthner Process

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Abstract

This study is devoted to CFD modelling of the gas flow and particle dynamics inside the reactor of a furnace used for regeneration of hydrochloric acid from iron chloride - a rest product from the pickling process in the steel industry. The understanding of the dynamics inside the reactor has shown to be of great importance in order to optimize the process. So far the process has been a black box, where only the inflow conditions are known together with the quality of the final product. In this work the gas flow is resolved together with the thermal distribution and the particle trajectory for the injected acid molecules.

Introduction

During hot rolling of thick metal slabs to thinner sheets in the steel industry, the surface gets oxidized by the surrounding air. Before the sheets are further refined in the production line these surface oxide films are removed in a process where the metal sheets are dragged through a pickling bath containing hydrochloride acid (HCl). Due to the formation of iron chloride ($FeCl_2$), HCl loses its ability to remove iron(II) oxide (FeO) from the surface. Hence fresh acid is continuously admixed to the container and the used acid is collected at the other end of the container [1]. Acid is hazardous to the environment and has to be regenerated which can be done by different techniques, such as spray roasting and different membrane techniques [2]. In a spray roasting reactor $FeCl_2$ is oxidized to iron(III) oxide (Fe_2O_3) and HCl is regenerated in a hot furnace. The hourly production/regeneration rate for such a process typically lies between five and ten cubic meters of acid.

Previous work about the process by Beck et. al. [3-4] has been focusing on the chemistry when drops of used HCl, H_20 and $FeCl_2$ forms Fe_2O_3 and HCl gas by the reaction

$$4FeCl_2 + 4H_2O + O_2 \rightarrow 2Fe_2O_3 + 8HCl + 55kJ\ . \qquad (1)$$

According to Beck et. al. [3-4] water evaporates from drops at 373 K until the mass fraction of $FeCl_2$ is 0.64 which corresponds to the mass fraction in Thetrahydrate ($FeCl_2 \bullet 4H_20$). The temperature of the drops increases and the water evaporates from $FeCl_2 \bullet 4H_20$ and is fully evaporated at 538 K.

The ideal reaction in (1) requires a ratio of H_20 to O_2 of 4:1 in the surrounding air. Otherwise several side reactions will appear which can be written as

$$12FeCl_2 + 9O_2 \rightarrow 6Fe_2O_3 + 12Cl_2 + 851kJ\ , \qquad (2)$$

when reduced to simplest form. This process has been modelled numerically by Beck et. al. [3-4], where the work in [4] also is validated with experimental data.

The present study focus on the flow characteristics in the process which is of importance to understand when optimizing of the process. Optimization parameters to be investigated involves changes of nozzle position, spray direction, size of droplets and power of burners. Optimization can be done in two ways: either by minimizing fuel costs or by achieve better quality of the particles.

This work is focusing on the initial two seconds after spray is introduced, which is the timescale of the vaporisation. After vaporization particles density will rise due to reaction (1) and (2). These changes in density is not modelled, therefore will particles only behave physical until vaporisation.

The spray roasting reactor used in the present study has a height of 18.5 m and a middle section radius of 4.3 m. The bottom part of the reactor is conical shaped with a height of 6.82 m and a bottom radius of 0.23 m. As viewed in Fig. 2 showing the cross section of the geometry, the main diameter of the reactor decrease fast close to the top of the reactor. Four natural gas burners placed tangentially to the reactor introduces heat for evaporation of the droplets, while the four spray nozzles feeding the system with used HCl are placed symmetrically at distance of 14.6 m from the bottom and at a radius of 1.5 m from the centre of the chamber. The nozzles are pointed 5° towards centre of the reactor. The droplets of acid from the nozzles have a mean diameter of 370 μm and has a mass fraction of 49 % H_20 and 51 % other substances, which are presented in Table 1.

1. Theory

1. 1. Governing Equations and Turbulence Model

The Reynolds Averaged Navier-Stokes equation is considered to govern the gas motion inside the reactor. As turbulence model, the Shear Stress Turbulence model (SST) which combines the k-ε and the k-ω model using a blending function, is considered. Far from the wall the k-ε model is used while the k-ω is used closer to the wall. The fluid is treated as non compressible.

1. 2. Liquid Evaporation Model

To calculate mass transfer due to evaporation, Antoine's equation is considered

$$P_{vap} = P_{ref} e^{\left(A - \frac{B}{T+C}\right)}, \tag{1.1}$$

where P_{vap} is the vapour pressure and P_{ref} the gas pressure, A, B and C are constants and T is the temperature of the droplets. If P_{vap} is higher than P_{ref} the mass transfer of water to steam is calculated using

$$\frac{dm}{dt} = \frac{-Q_C}{V}, \tag{1.2}$$

where Q_C is convective heat transfer and V the latent heat.

2. Numerical modelling

2. 1. Geometry and Mesh

Some simplifications of the geometry are considered in order to simplify the mesh generation and the calculations: i) The lances which holds spray nozzles are neglected. ii) wall - which in reality is made of bricks and hence imply a non-zero value of the surface roughness - is treated as smooth (i.e. the surface roughness is not considered).

In order to obtain reliable results a mesh of good quality and which have sufficient number of nodes is crucial. Here the region close to the burner is meshed with tetrahedrals due to sharp angle in geometry while the rest of the domain is meshed with hexahedral elements. To verify that enough number of nodes were used a mesh analysis was made, see Fig. 1.

2. 2. Boundary Conditions

Each of the four burners is fed with natural gas and air: 71 nm^3/h and 2240 nm^3/h respectively, where nm^3/h is normal cubic meters per hour. This corresponds to a mass flow of 0.83 kg/s. The water mass fraction is set to 0.1. The temperature of gas is 1040°C, which is measured continuously in the process. The flow is simulated as non compressible.

The four nozzles has a spray angle of 60° and are simulated as point sources with the given spray angle. The droplets are considered normal distributed with a mean diameter of 370 μm and a standard deviation of 100 μm. The initial velocity is 13 m/s and the temperature is set to 60°C. Through the nozzles 1200 particles is introduced and tracked during the simulations. Eulerian-Langerian approach is used for particles tracking the coupling between those is two way so evaporated water from particles will be transferred into the continuous phase. Forces acting on particles in simulations are buoyancy and dragforce. The heat transfer coefficient for the wall is set to 0.6 W/m^2K. The evaporation is calculated from (1.1) using values of the constants such that A=5.11564*ln(10), B=1689.54*ln(10) and C= -65.15 [5]. The density of the other products than water is set to 1500 kg/m^3 to fulfil the initial condition of acid density which is 1240 kg/m^3. When the particles starts to react with O_2 and H_20 the density will rise in reality which is not implemented in this model. The two stage evaporation process described in [2] is not considered in the present study but is a highly interesting development to be treated in the future. Tab. 1 shows the exact composition of the used acid.

Tab. 1. Mass fraction of substances in acid

Substance	Fe^{2+}	Fe^{3+}	HCl	Cl^-	H_20
g/l	204	28	39	362	607

3. Results and Analysis

3. 1. Mesh Analysis

Mesh analysis of three different grid spacings are compared: 280,000, 780,000 and 1,700,000 nodes respectively. Simulations are made with the final model, with heat loss and evaporation included. Respectively results are compared in Fig. 1, showing no significant difference in temperature or mass fraction. The final simulations have been done using the 780,000 nodes mesh.

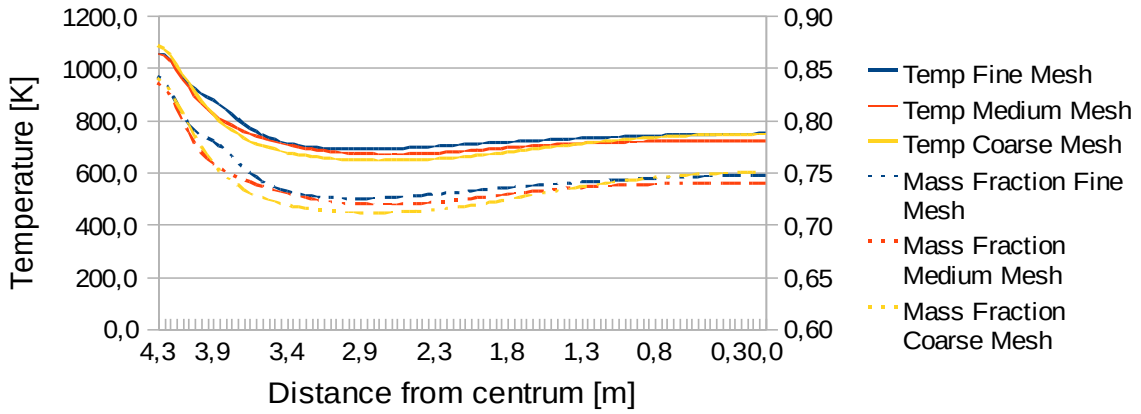

Fig. 1. Mesh analysis of temperature and mass fraction of air along a line perpendicular to wall

3. 2. Character of Flow

In Fig. 2 the temperature distribution and velocity profile is shown. The velocity is directed upwards close to the wall, while it makes a rapid change with a dominantly downward direction at distance of 0.3 m from the wall, with another change of direction in the middle of reactor. This profile can be explained by the temperature distribution with hot air from burners rising along the wall, while in the region of high temperature gradient, the flow changes in direction and moves towards the bottom of the reactor.

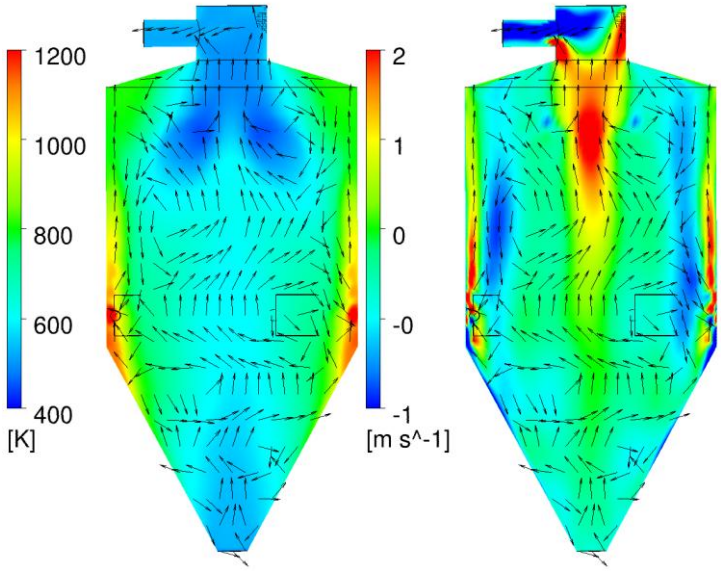

Fig. 2. Left: temperature distribution. Right: velocity profile in vertical direction. Arrows with equal length shows direction of flow in the plane

3. 3. Validation of Numerical Model with Measurements

The temperature profile has the same characteristics in both cases, with highest temperature 0.1-0.2 m from the wall and temperature change in the same region. The difference in temperature in the region close to the wall can be explained by a low valueof the specific heat for the acid. Furthermore, measurements capture the convection from the colder walls

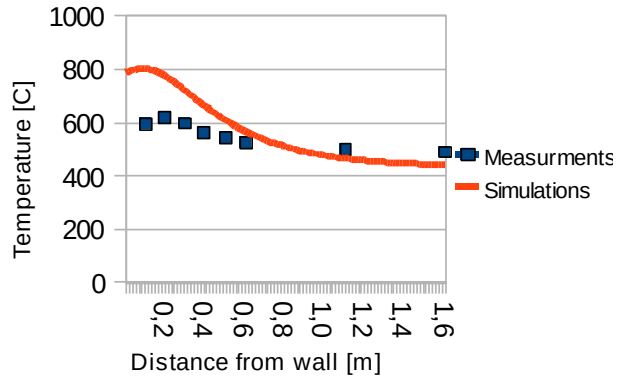

Fig. 3. Comparison between simulations and measurements. Temperature is taken along a line, 1 m above burner, perpendicular to wall

which could affect the accuracy of the measurements. Also , the temperature of the exhaust gas could have been set too high due to a high temperature on the burner walls which results in convection heat to the thermoelements placed in the burner chamber.

3. 4. Droplet Evaporation

In order to optimize the Ruthner process, one parameter to vary is the nozzle position. The results in Fig. 4 is taken two seconds after injection, showing that particle evaporation and distribution is changing with nozzle position. With nozzles placed close to the centre, droplets tends to stay in upper part longer with a slower evaporation as result. Having nozzle position close to the walls makes the droplets travel faster in vertical direction and evaporation is slightly faster compared with the position 1.5 m from the centre.

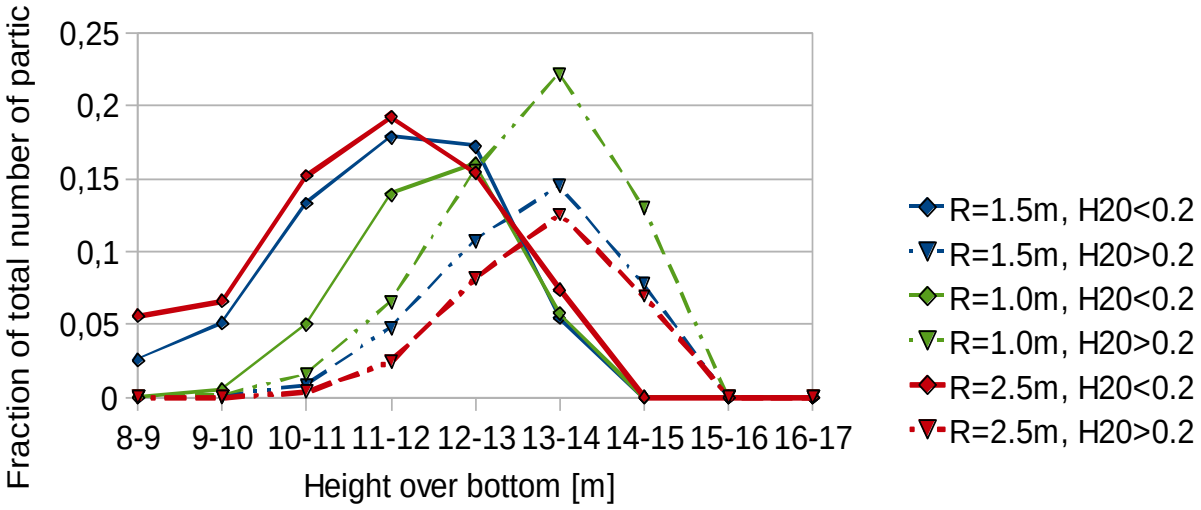

Fig. 4. Particle evaporation depending on placement of nozzle at radius 1.0, 1.5 and 2.5 m from centre. Dotted line: is particles containing less then 20% water. Solid line: particles containing more than 20% water. Particle distribution two seconds after injection

4. Summary and Conclusions

In this study the flow characteristics of a spray roaster furnace has been investigated numerically. The physical models that has been introduced to the simulations are evaporation, heat losses thorough walls, drag force on particles and the dynamics of the gas flow. It is shown a dramatical change in direction for the vertical velocity when going from the boundary wall towards the centre of the reactor. This is caused by sharp temperature gradients, leading to significant density variations and dominant buoyancy effects within the gas flow. These fluctuations play a key role in the overall dynamics of the gas flow inside the reactor, and hence also for the whole regeneration process. A comparison between modeled temperature

and data from measurements reveal a good correlation in the inner region. Also the characteristic of the the two are good, with the highest temperature at distance 0.2-0.3 m from wall and the highest temperature gradient in the same region. It is also been shown how the time of evaporation is effected by the nozzle position.

The numerical model presented in this paper gives a good idea of the flow and distribution of temperature in the process representing the droplets until evaporation. To give the full picture of particle distribution however, density change of particles has to be introduced. This can either be done by implementing the full chemistry model or by setting a mass exchange between gas and solid, as a function of time and temperature. An uncertainty in these simulations is the heat capacity of the solid part of the particles, here set to 460 J/kgK wich corresponds to the value of iron oxide.

When monitoring the solver, fluctuation in velocity and temperature is seen. This can be explained by transient effects in the process. These effects can be captured by running transient simulations, which are very time consuming. Steady state simulations are therefore to prefer and is a good trade-off between quality and time.

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