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COMPUTATIONAL STUDY OF DYNAMICS OF DROPLETS

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Abstract: Spray roasting of metal chloride solutions in spray roasting reactor is usually done in steel industries to recover pickling liquids. This spray roasting reactors are very difficult to characterize experimentally, because of their large size and high operating conditions. So computational fluid dynamics simulations have been used to analyze reactor performance. These CFD simulations require a particle formation model, this model then describe the particles size history including the characteristic effect of particle swelling. The influence of particle swelling on the process is also discussed. The results clearly indicate the necessity to investigate particle swelling, potential collision effects of spray roasting reactors. There is a need to better understand the dynamics inside the spray roasting reactor, which in turn will improve possibilities to optimize the spray roasting process. In this project velocity, temperature distribution, water vapour and HCl gas concentrations throughout the reactor are numerically modelled together with the droplet motion inside the reactor. These were modeled before and after changing spray nozzles positions to investigate the effect of it on the flow characteristics of the continuous and dispersed phase, and the relation between temperature and energy efficiency and the regeneration process. For model setup or design of spray roaster geometry, mesh, boundary conditions, burner inlet specifications, all these specifications are defined in this work.

1.INTRODUCTION

Hydrochloric acid has been widely used as pickling liquor for hot steel surfaces. During the pickling process hydrogen chloride reacts with iron oxides and forms iron chloride ($FeCl_2$). The pickling speed gets reduced by this enrichment. After reaching a critical concentration of $FeCl_2$, the spent pickling liquor has to be recovered. To recover this pickling liquid spray roasting reactor is used. In this type of reactor $FeCl_2$ solution is injected with water through one or more nozzle holders.

Each nozzle holder comprises of a number of single fluid pressure spray nozzles. Gas burners are usually used to supply the thermal energy which is required to evaporate the water contained in the solution, which is roughly 3MJ per spent of pickling solution. The burners are mounted tangentially which creates a rotating gas flow within the reactor causing effective mixing. Because of which the vortex formation takes place which helps to increase the residence time of the particle injected and consequently supports sufficient chemical conversion. The thermal decomposition process leads to HCl, which is returned into the pickling process through the exhaust outlet on the top of the reactor. Because of the gravity the Fe2O3 (hematite) particles leave the reactor through the particle outlet at the bottom of the reactor.

The Fe2O3 is a desired byproduct which is useful in different industrial process like ferrite or pigment production. Therefore, no chlorine should be contained in the roasted iron oxide to provide a product of high purity and also, only Fe2O3 is preferred as iron oxide. And the undesirable oxides are FeO and Fe3O4, which are results of incomplete roasting while the formation of γ- Fe2O3 is caused by too high temperatures. The chemical reaction of the recovery process of FeCl2 is given by

$$4FeCl2 + 4H2O + O2 \rightarrow 2Fe2O3 + 8HCl - 55{:}0 \text{ kJ/mol}$$

The chemical reaction is exothermic, the process requires additional energy input , as the spent pickling solution roughly contains 70% of water by weight. But due to their large size and particle laden, aggressive and high operating temperatures of the industrial scale reactors measurement are extremely difficult. And also the experimentally based information on details of particle formation in the different zones of the reactor is very limited, so a very attractive is CFD modeling of these reactors.

2. Theoretical background

The spray roasting process which is used for regeneration of the FeCl2 are divided into several steps which involves the conversion of FeCl2 into solid iron oxide particles.

The steps are as follows:

- Inert heating of droplets: The droplets which are injected into the reactor from the spray nozzle holders on the top are first heated to the boiling point of the water.
- Boiling: Iron chloride forms hydrates at the surface of the droplets because of which some amount of water is bound to the surface and on boiling the free water gets evaporated at 373 K. -Transformation to a hollow sphere: During this evaporation process, iron chloride stays at the surface of the droplet, while the free water gets evaporated this leads to the increase in concentration of iron chloride on the droplet surface. But when this concentration reaches a critical value, no more water can evaporate from the surface i.e. the surface becomes impermeable. But there still some amount of water remaining inside the particle, and the further evaporation lead to increase in the pressure inside the particle. This causes the swelling of the particle and leads to a hollow sphere.

• Drying of hydrate water: After the free water on within the particle has evaporated, the water bound to FeCl2 starts releasing. This occurs in a stepwise manner through a number of iron chloride hydrates: FeCl2 · 4H2O to FeCl2 · 2H2O at 379 K, FeCl2 · 2H2O to FeCl2 · H2O at 433 K, and finally FeCl2 · H2O to FeCl2 at 538 K). When the monohydrate is converted to the pure iron chloride, the formation of iron oxide(Fe2O3) starts.

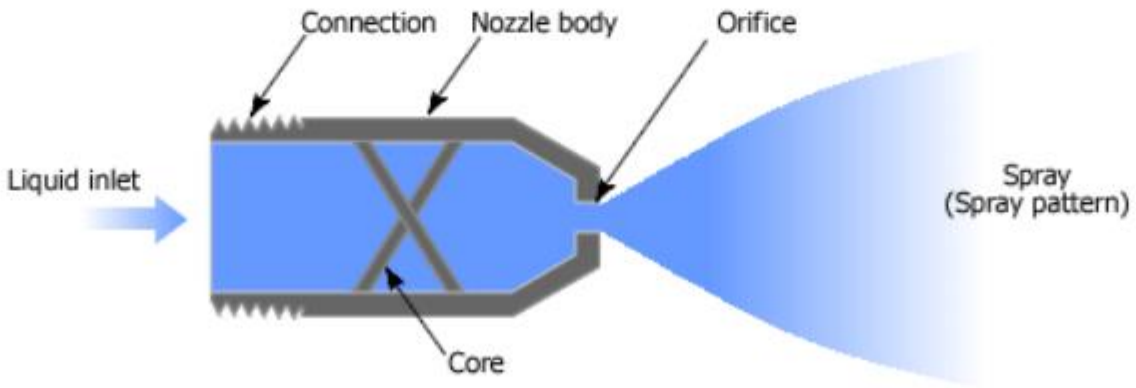
• . The reactions are as follows: [1] $4FeCl_2 + 4H_2O \rightarrow 4FeO + 8HCl$ +508 kJ/mol (1) $4FeO + O_2 \rightarrow 2Fe_2O_3$ −563 kJ/mol: (2) In the first reaction, the chlorine is split of and HCl is formed, while in the second reaction, the desired Fe2O3 is created by further oxidation, so the two processes by the consumption of H2O with simultaneous release of HCl and the oxidation process takes place in one step each. As reactions (1) and (2) require gaseous reaction partners (H2O and O2), the net reaction rate is influenced by three mechanisms: boundary layer diffusion, pore diffusion, and chemical reactionkinetics Pore sizes of 4–5 nm were found to be dominating, which causes the process to be dominated by pore diffusion

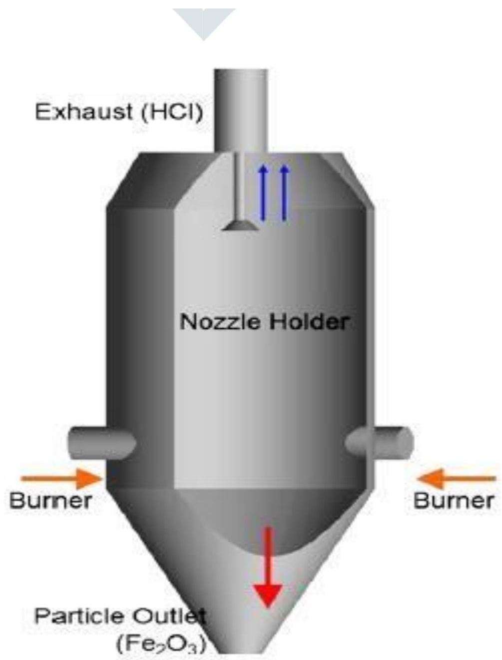
3. Position of Nozzle in spray roasting process

In terms of the energy efficiency of the drying process, the outlet temperature is a valid indicator. In Table 1,results are presented for the outlet temperature for three nozzle positions. It found that almost indistinguishableresults were obtained when the nozzle position are r = 0.5 m and r = 1.5 m respectively, while a higher outlettemperature is obtained when the spray nozzles are located at r = 3 m. The reason behind this result is that thenozzles are now placed closer to the wall, the particles will have limited region to evaporate close to the wall, so temperature close to the wall will drop due to droplet evaporation and will cause cold air sink through the process

, because of this heat loss also get reduced through the wall.

As these nozzles are placed close to the centre, after changing setup the water vapour concentration is also changed Aclear difference is visible as compared to the reference. The highest concentration of water vapour in the reactor is found directly below the exhaust with a fraction of more than 30 mol%. In all other parts of the reactor, the water vapour concentration values are between 18 and 25 mol% which are very minor gradients. The water vapour is transported to the lower part of the reactor with the help of large vortex that rotates in the opposite direction compared to the reference configuration and it also initiates effective mixing in the reactor





4. Numerical Calculation

A model was developed for the spray roasting process of iron chloride solution to analyse the particle formation and reaction within the reactor. This model was implemented in ANSYS Fluent. When a droplet of particle is heated to the boiling point of water (T = 373 K), the unbound water evaporates from that particle, which leads to a reduction in droplet size and an increase of the density[2].

$$\frac{d}{dt}d_p = \frac{4\lambda}{\rho_p c_{p,g} d_p}\left(1 + 0.23\sqrt{Re_p}\right)\ln\left[1 + \frac{c_p\left(T_g - T_p\right)}{h_f}\right] \quad -(3)$$

Where ρ_p is droplets density, $d_p$is diameter, $T_p$is temperature, $cp,_g$is the heat capacity of the surrounding gas phase, and h_f the latent heat of water. Eq. (3) whichis based on the Nusselt number correlation Nu=2+√Re^3√Pr Note that while evaporation of the unbound water, the particle temperature is assumed to be constant i.e. the temperature gradient in the particle, which may develop in larger particles, is neglected here.

The evaporation process leads to a change in the droplet composition in the reactor. As there are no distinct formulations which give the relation of the dependence of the density of a mixture of the different iron chloride hydrates that occur during the further process, so the density of the particle at a given time is calculated by a mass weighted approach:

$$\rho_p = \frac{1}{m_p}\left(\sum_i m_i \rho_i\right) \quad (4)$$

Here, mp is the particle mass, mi is the mass of the ith component, and ρi is its density. Note that this model used for the density calculation, only differentiates between unbound water, water bound to iron chloride tetra hydrate ($FeCl_2.4H_2O$), pure iron chloride ($FeCl_2$), wustite (FeO), and hematite (Fe_2O_3)[2].

As the evaporation process proceeds enrichment of $FeCl_2$ in the outer shell of the droplet starts to occur i.e. the concentration of $FeCl_2$ starts increasing in the outer shell of the droplet. When the outer shell consists of 64% of $FeCl_2$, i.e., pure iron chloride tetra hydrate, an impermeable shell is formed and particle swelling starts. For the particle diameter growth, it is assumed that the forces are caused by the pressure of the vapour within the particle and by surface tension are in equilibrium.

$$\frac{\pi}{4}p_i d_i^2 = \pi d_p \sigma s.$$

5. Modelling industrial scale reactors

The reactor recycles 6 m^3 of spent pickling liquid per hour. Four tangentially mounted burners are used as energy supply to the reactor and to guaranty the swirling of flow within the reactor[1].

In this project, two configurations are taken with different locations for the two nozzle holders, each holder holds 14 nozzles each, which are then are compared. In the first setup which is also used as reference configuration in that the two nozzle holders are placed at a distance that measures 16.6% of the reactor diameter from the centerline of the reactor; in the second case, the nozzle holders were placed in a distance that measures 10.6% of the reactor diameter from the reactor centerline. In both cases, the injection was placed at the same height, which is approximately 80% of the vertical height taken from the reactors particle outlet (bottom). The spray angle of each nozzle was set to 22.5° towards the centerline, and the initial droplet velocity from the nozzle was set to 10 m/s. A Rosin–Rammler particle size distribution was fitted to the data, yielding $Y= 1-\exp(-(d/375.2)^{2.43})$ where Y denotes the cumulative particle volume fraction and d is the particle diameter in micrometers.[1]

The energy required for this complete regeneration process is 2.9 $MJ/l_{solution}$ .The reactor was fed with 4,135 m^3/h solution with a concentration of 28.9 wt% of $FeCl_2$ and a density of solution is 1368 kg/m^3. The parameters of the gas flow through the burners are summarized in table

Table . Burner feed conditions for setup

	Air	**CH_4**
T (°C)	**25**	**25**
V(Nm3/h)	**8361**	**525**
Mass flow/burner (kg/s)	**0.961**	**-**

6. Result & discussion

The work presented shows that how changing the position of nozzle holders can influence the efficiency of the spray roasting reactors, when the iron chloride solution is injected it was seen that it affects the gas phase properties like temperature, flow field, and concentration. To analyze it, differences in the behavior of the discrete phase in the reactor were calculated. This results showed that the change in nozzle holder location causes severe influence on the performance of the reactor.

Two model was simulated first case was taken as reference reactor with nozzle holder position measuring 16.6% of the reactor diameter from the centerline and in second case, nozzle holder were placed at a distance measuring 10.6% of the reactor diameter from the centerline.

This change in nozzle holder distance caused serious change in the temperature profile of the gas phase. The temperature profile in the first case colder zone was much enlarged than in from the second case. In total the temperature profile is more homogeneous than in the first case, with average temperatures of 1000–1100 K in the entire reactor.

Also it is observed that the tangential component of the gas velocity is slightly higher, especially close to the reactor centre. The core vertical vortex is now shifted upwards and much closer to the centerline. In addition, the gas phase is now transported to the upper part of the reactor due to the vortex rotating in the opposite. Instead of our initial assumption, which has led us to change in the configuration, the ascending gas flow between the nozzle holders has not been reduced. An ascending gas flow close to the reactor wall is still visible.

In second case the highest concentration of water vapour is found directly below the exhaust having concentration more than 30 mol%. In all other parts of the reactor, the water vapour concentration values are between 18 and 25 mol%. The water vapour is transported to the lower part of the reactor with the help of large vortex that rotates in the opposite direction compared to the reference configuration and it also initiates effective mixing in the reactor.

The HCl release to the gas phase is also affected by the change in nozzle holder position. The highest HCl release rates are shifted upwards, which shows that particles are transported to the upper reactor part by the core vortex

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