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CFD Assisted Scale Up of a Rotating Drum Leaching Reactor

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During the development phase of a new technology it is inevitable to define different scales from laboratory through pilot to industrial level. The information transfer between these levels is crucial, because similar yields and conversions should be achieved in an industrial scale device, which were obtained in a laboratory scale reactor. To maintain the same performance the construction and operation parameters are often changes during the scale up procedures.
The scale up of a mechanically stirred reactor is especially challenging since similar conditions are difficult to recreate at higher scales. Traditionally dimensionless numbers can be used to calculate the proper operating parameters and sizes for the new reactor, ensuring the proper conditions. However, a validated CFD simulator can be an excellent tool to perform scale up studies with less resource needed.
This work is aimed at the scale up procedure to support building a pilot plant scale leaching reactor, used for the dissolution of metals form waste electric and electronic equipment. Particularly the process deals with the dissolution of copper which has the second highest economical potential after precious metals. The laboratory scale leaching reactor and its validated CFD model were developed and discussed in detail in a previous study. The scale up studies is based on the validated model of the laboratory scale reactor. Different construction and operation parameters were tested using CFD simulations. Based on the flow rates from the CFD simulations we calculated the component balances and conversion using a compartment model. Similar hydrodynamic conditions can lead to the same conversions, and product yields, but at a higher scale. For the modelling studies COMSOL Multiphysics will be used as CFD software and MATLAB for conversion and utility calculations.

1. Introduction

One of the most important steps in the development of a new technology is the scale up procedures, to transfer information from the laboratory scale to the pilot and industrial plant scale. The scale up procedures was emerged as a new field of science due to their complex nature. Dimensionless numbers are widely used in the field of chemical engineering, for design and development purposes (Ruzicka 2008). With the dimensionless number the similarities between the different scales can be ensured, and scale up calculation can be completed. However, the computation can be complex and time consuming and does not always ended with the expected results (similar operation). Computational Fluid Dynamics (CFD) methods can be an excellent way to support the scale up procedures. Using a validated CFD model the laboratory scale results can be transferred easier to pilot plant, and higher scales.
CFD simulators can be used in different scale up applications in different industries. In the pharmaceutical industry, one of the most crucial aspects is the purity of the product to ensure the proper quality (Muller et al., 2009). The development are often start at laboratory scale, and the scale up lasts to industrial scale through pilot scale using batch operating devices. In the crystallization processes the laboratory scale device is usually a 1 L vessel, the pilot plant devices are 100 Ls to 1 m^3, and even larger devices are used in industrial scale. The problem in the scale up in case of crystallization is the average particle size which

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can be different in every scale. Besides during the scale up procedures different heating and cooling profiles can be applied (Paul et al., 2004). With a detailed CFD model the morphological changes, and the hydrodynamics inside the crystallization device can be accounted for, and using a CFD simulator the time of the development can be reduced. Using computer aided methods, compartment, and CFD models a real crystallization device can be created in a full 3D simulation. With the modelling of the heating and cooling, the operation of the device can be modelled, and the different scale vessels can be compared to each other. With the help of the simulator the same yield can be recreated in higher scale which will lead to the next scale, or ultimately the building a new plant, based on CFD models (Wei et al., 2010). Besides of the industrial scales the scale up procedures in the pharmaceutical industries often means to achieve a pilot level, or a smaller bioreactor in industrial scale (10-100 Ls). These reactors are often used in vaccine development (Hundt et al., 2007), or in the development of new pesticides (Hameed, 2001).

Different mechanical stirred reactors are used in the industry. These devices are often facilitates multiple phases (gas, solid and liquid), so a multiphase model often be a correct choice for modelling these systems. Some of the reactors contain multiple impellers in one shaft. If the reaction mixture is disposed to foaming an anti-foam impeller can also be used besides the normal Rushton turbines (Takesono et al., 2006). Mathematical model based method is an excellent way to perform the scale up procedures of a vinegar producing fermentation (Gonzalez-Saiz et al., 2009), including cooling, economical and optimisation studies too. However, the application of model based methods in design can be excellent way not only gas-liquid, but other multiphase systems (e.g. slurry reactors (Montante et al., 2003)).

CFD simulators can be an excellent tool to do the scale up calculations even in multiphase systems. The CFD supported scale up process can be divided to three different steps:

1. Define the exact 3D models of the devices of different scales (laboratory, pilot, plant size).
2. Solve the models, and compare the possible alternative configurations at different scales based on the results.
3. Make modifications of the higher scales; try to recreate similar conditions (for example changing the number, angle, position or type of the impeller).

With this CFD supported scale up process the higher scale device can be developed capable of producing the same yield, and conversions, than in smaller scales (Gentric et al., 2005).

In this study a CFD model based scale up method was developed. A case study of chemical leaching reactor was used.. A copper leaching reactor was chosen, because copper recovery is one of the most prosperous processes in the field of electrical and electronic waste recycling technologies (Fogarasi et al., 2013). The reactor contains a rotating perforated drum, and the leaching reactions have taken place inside the drum. The laboratory scale device and the model of the device were developed in our previous research, connecting a CFD model and a heuristic compartment model (Egedy et al., 2013). Different geometries were implemented in CFD software, and using the simulation results conversion values was calculated. The goal is to recreate the same conversion, which we obtained in case of the laboratory scale device. Besides the CFD based a traditional scale up calculation was completed. The obtained results were evaluated, and an optimal reactor configuration was proposed. COMSOL Multiphysics was used for CFD simulations and MATLAB for the conversion calculation.

2. Modelling, and scale up procedures

Two different approaches were used for scale up a leaching reactor with a rotary drum. The traditional methods are not able to take account on the other geometrical factors (e.g. the number, the diameter, the positions of holes on the drum, etc.). A CFD based method was proposed to calculate with these factors. Different larger scale reactor configurations were implemented based on different constructional parameters.

- Hole number from 2 to 6 in one row (8 rows)
- Hole diameter from 2 cm to 5 cm
- Drum diameter (0.3, 0.4, 0.5 m)

Sum of 30 geometries was examined. Table 1 shows the identification of the different cases. A copper leaching reaction was implemented for the scale up studies using $FeCl_3$ as reagent (Eq(1) and Eq(2)). The kinetic identification was presented in detail by Popescu (2013).

$$Cu + 2Fe^{3+} \rightarrow Cu^{2+} + 2Fe^{2+} \quad (1)$$

$$Cu + Cu^{2+} \rightarrow 2Cu^{+} \quad (2)$$

Table 1: The investigated case studies

Case No.	Drum diameter [m]	Number of holes	Diameter of holes [m]	Case No.	Drum diameter [m]	Number of holes	Diameter of holes [m]
1	0.5	2	2	**16**	0.5	2	3
2	0.5	3	2	**17**	0.5	3	3
3	0.5	4	2	**18**	0.5	4	3
4	0.5	5	2	**19**	0.5	5	3
5	0.5	6	2	**20**	0.5	6	3
6	0.4	2	2	**21**	0.5	2	4
7	0.4	3	2	**22**	0.5	3	4
8	0.4	4	2	**23**	0.5	4	4
9	0.4	5	2	**24**	0.5	5	4
10	0.4	6	2	**25**	0.5	6	4
11	0.3	2	2	**26**	0.5	2	5
12	0.3	3	2	**27**	0.5	3	5
13	0.3	4	2	**28**	0.5	4	5
14	0.3	5	2	**29**	0.5	5	5
15	0.3	6	2	**30**	0.5	6	5

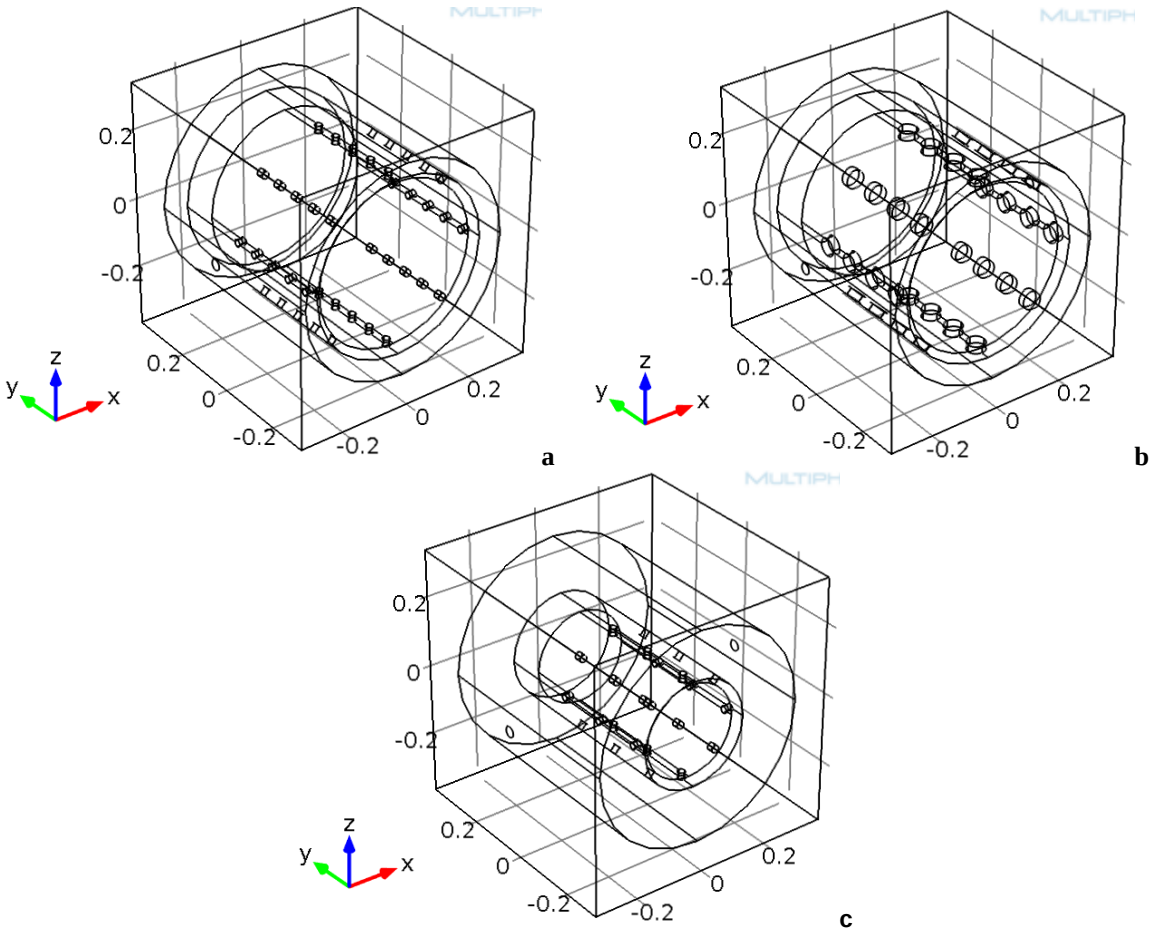

Figure 1 a) 5-hole construction with 2 mm hole diameter and 0.5 drum diameter (case 4), b) 4-hole construction with 5 mm hole diameter and 0.5 drum diameter (case 28) c) 3-hole construction with 2 mm hole diameter and 0.3 drum diameter (case 12)

Figure 1 shows some of the implemented geometries. Momentum balance was solved for each of the implemented models, and using the flow rates calculated from the velocity vectors a compartment model was defined (hybrid CFD-compartment model).

The compartment model was used to calculate component balances in the reactor. The model descriptions are discussed in details in Egedy et al. (2013).
After the hybrid models were built a copper leaching reaction was used to test the effectiveness of the constructions. All the simulations were performed for 2 h. Then the comparison of different constructions was evaluated by using the leach effectiveness (basically a conversion of the copper from the solid phase). Based on the achieved results an optimal construction was proposed for the larger scale.

3. Results and discussion

Based on the similarity of the flows the literature suggests the following formula to calculate the diameter and the revolution speed for the industrial scale vessel, based on the laboratory scale (Paul et al. 2004).

$$d_l \cdot N_l = d_p \cdot N_p \tag{3}$$

In Eq(1) d refers to diameter, N to revolution speed, the subscript l as laboratory and p to pilot scale. However, our case is specific because

- The impeller geometry is specific (basically a drum).
- The drum is perforated.

The basic equation does not contain any suggestions to handle perforated or specific impellers. It was developed for basic impellers (blade, turbine, anchor etc.).The geometric parameters of the laboratory scale device were 0.05 m diameter, and 30 min^{-1} revolution speed was applied. In the next scale the diameter of the drum will be 0.5 m, and the calculated revolution speed is 3 min^{-1}. Applying this revolution speed, the similar flow conditions (Re number etc.) can be ensured (case 31). The experimental apparatus is not suitable for such low revolution speed, so we used the simulator to test the results.
An 8 core computer was used for the calculations with 72GB memory. The computations lasted from 3 up to 9 days per case. The similarity of the reaction was guaranteed as the same molar composition of oxidant is used, and the ratio of the metal, and the solvent was the same. In the final step of the simulation the conversions were calculated. Beside the basic case (0.3 M concentration of $FeCl_3$ reagent 30 min-1, 0.1 L/h inlet flow rate), the flow rates and the concentrations were changed, and a sensitivity analysis was evaluated. Figure 2 shows the results of the sensitivity analysis for 0.3 M reagent concentration.
Case 31 is applied as a reference case. The parameters are the same in every this is the only case when the flow rates do not change. The reactor geometry is similar to the laboratory scale device, and the hydrodynamic similarity was ensured. The flow rate was the same in case 31, because changing the flow rate will change the hydrodynamic conditions inside the reactor, so the similarity between the laboratory and pilot scale device will change to. Practically case 31 is evaluated with one flow rate while the other cases were evaluated with ten flow rates.

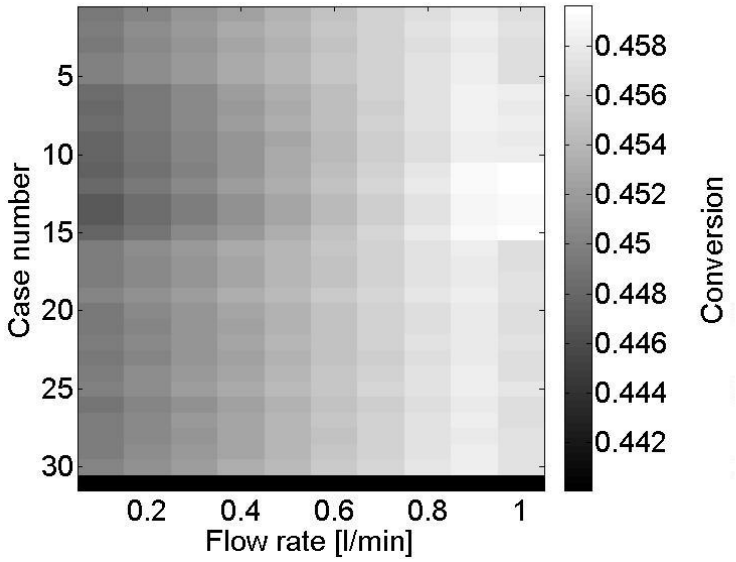

Figure 2: The obtained copper conversion at different reactor configurations using 0.3 M $FeCl_3$ concentrations

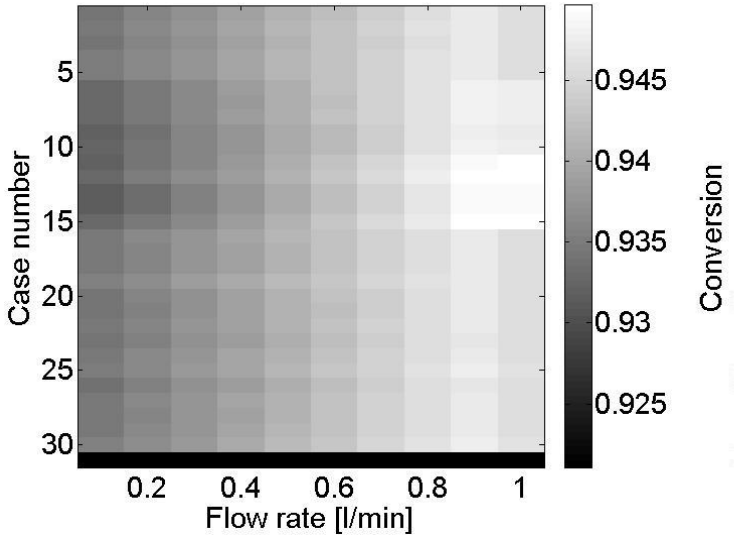

Figure 3 The obtained copper conversion at different reactor configurations 0.6 M $FeCl_3$ reagent concentrations

As Figure 2 shows at lower flow rates there are smaller differences between the cases, however all the cases with changed geometries are more effective, than case 31. At lower reagent concentrations a maximum of 2 % increase can be achieved by manipulating the geometry, and construction parameters of the leaching reactor. In the next examination a higher reagent concentration was applied (0.6 M). Figure 3 shows the results, the conversion values of the different cases with different flow rates compared to case 31.

With higher reagent concentrations almost 3 % increase can be achieved by manipulating the geometry. The obtained conversion values are lower than we achieved in the laboratory scale, but using the hybrid CFD-compartment approach the performance of the reactor can be increased by changing the geometry before creating the higher scale device. As Figure 2 and 3 shows the highest concentrations can be achieved by applying the case 15 geometry, the lower drum diameter, and higher number of holes.

4. Conclusions

A CFD assisted method was used to design a higher scale leaching reactor, using a hybrid CFD-compartmental approach. Different geometries were compared to each other based on conversion values. The results shows that the CFD assisted scale up methods can increase the effectiveness of the basic scale up methods. Based on the achieved results geometry was proposed (case 15) for the pilot plant scale device.

However, the technology is still in the development phase and using CFD simulators other analyses should be taken place, e.g. the examination of the revolution speed dependence of the conversion in the pilot scale device.

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