Modelling of NO Oxidation in a 3D-Printed Catalytic Foam Reactor

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Highlights

- EU project PRINTCR3DIT. Innovative reactor concept using 3D printed artificial foams
- Complex model of a fixed bed reactor using 2D (axial, radial) bed and pellet model
- Catalyst mass transfer is included in the reactor model
- Optimization of design and operating point for pilot plant setup

1. Introduction

In the EU project PRINTCR3DIT, including 13 participants from R&D centers, universities and industry, innovative reactor concepts have been analyzed. One focus is the use of 3D printed iso-rectangular foams for reactor design. A NO oxidation reactor has been analyzed. This reactor is part of an Ostwald plant for nitric acid production, operated by Yara. Besides high conversion and efficient heat integration, low pressure drop is a major design goal.

2. Methods

Kinetic experiments for the catalyst, pressure drop experiments for a variety of foam geometries and heat transfer measurements have been performed. Experimental work was done in a differential bed reactor. This data is then used to adapt kinetic equations and pressure drop and heat transfer correlations. In conjunction with thermodynamic methods like gas properties and equilibria these parameters represent the input for a sophisticated fixed bed reactor model. The catalyst bed model is capable to depict axial and radial concentration and temperature profiles in the tube side. A shell side model describing co- or countercurrent flow can be attached. The catalyst bed model can be used in pseudo-homogeneous mode. Alternatively, the solid catalyst is numerically resolved using an approach derived from the dusty gas approach [1], modified for improved numerical properties. The mass, heat and momentum balances describing the reactor performance are solved using an in-house code which is capable to solve the model equations very efficiently.

3. Results and discussion

As expected for exothermal equilibrium reactions the heat release drives the system towards equilibrium limitations, therefore heat needs to be removed continuously while the reaction progresses. The design goals are contradictory, as simultaneously low pressure drop is required as well as high conversion with effective heat recovery and thermally stable operation. This implies the necessity for low local temperature difference for heat transfer, i.e. high heat transfer coefficients. To achieve this at low pressure drop, a packed catalyst pellet bed is replaced by a 3D printed iso-reticular structure with porosities higher than 90%. A typical example of the 3D printed structure is shown in Figure 1.

A countercurrent cooling heat removal is designed as a sensible heat sink by a cooling medium to achieve the desired temperature profile and evoking partial evaporation to limit the shell side pressure. A typical simulated profile is shown in figure 2.

The evaluated operating point will be implemented in a pilot plant reactor.

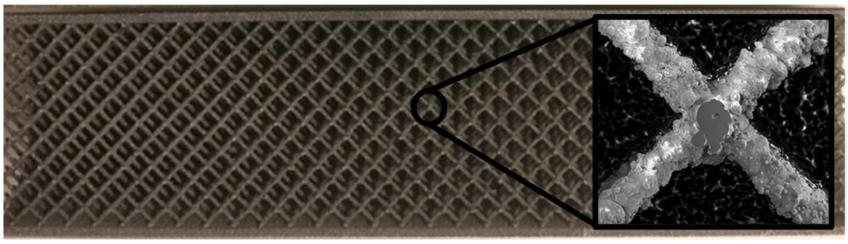

Figure 1. Example of a 3D printed iso-reticular fam with cubic unitary cells.

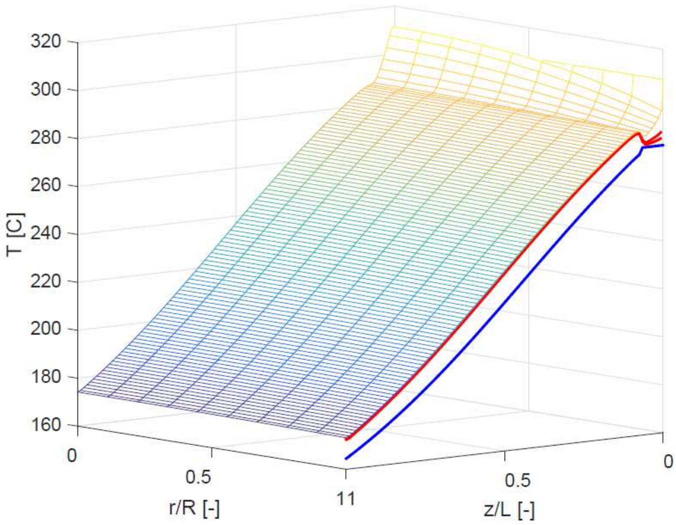

Figure 2.: Example reactor temperature profile with bed profile (contour), wall temperature (red) and cooling medium temperature (blue)

4. Conclusions

It was shown that a printed foam is an alternative to a pellet bed for exothermal equilibrium reactions with the advantage of a significantly reduced pressure drop.

On the modelling level, it is emphasized, that with simple model variations like algebraic variable transformations and sound simplifications, the numerical efficiency can be dramatically improved. The presented model converges within seconds on a standard PC.

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References

[1] R. Taylor, R. Krishna, Multicomponent Mass Transfer, Wiley, New York 1993.

Keywords
"Fixed Bed"; "Reactor Model"; "Catalyst Model"; "Ostwald Process"