**Development of an intensified heat exchanger reactor manufactured by 3D printing for acrolein synthesis.**

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**Highlights**

* The catalytic oxidation of propylene into acrolein is studied.
* Kinetic parameters are identified by optimization.
* A milli-channels heat exchanger reactor is developed to intensify heat transfer.
* Numerical validations by CFD calculations are performed.

**1. Introduction**

Acrolein synthesis is a key stage in the multi-step methionine production process, which is an amino acid used as a nutritional additive for animal feed. Acrolein is produced by heterogeneous and exothermic catalytic oxidation of propylene in gaseous phase. Numerous side reactions can occur leading to a moderate acrolein yield. The conventional industrial reactor is a multitubular fixed bed cooled by molten salt. The axial temperature profile in tubes presents a quite large hot spot which is partly responsible for the promotion of side reactions. The use of an intensified milli-channels heat exchanger reactor (HEXR), in which the catalyst is wash-coated on the wall, is then required especially to better control the temperature profile and to avoid the use of hazardous molten salts. Besides, additive manufacturing offers the opportunity to develop new HEXR configurations and to avoid solder joints by manufacturing the device in one unique piece. Then, the HEXR is built by metal 3D printing. This work consists in:

* the determination of a precise kinetic model to enhance catalyst performance prediction,
* the sizing of the new milli-channels HEXR,
* the validation of the device by CFD calculations.

**2. Kinetic modelling**

The first step of the work is therefore to improve the prediction of the kinetic model with respect to the experimental data. A first reaction scheme was established by Arntz *et al.*1 from measurements of initial formation rates of products. A more complete kinetic model, containing 10 species and 10 chemical reactions, was also developed by Redlingshöfer *et al.*2. A new kinetic model was then established by taking into account information from literature and experimental observations. This kinetic model considers the propylene adsorption and the oxidation ratio of the catalyst surface. Experimental data were collected on a catalytic screening platform consisting in isothermal fixed bed reactors coupled by on-line gas chromatography. Influences of temperature, gas hourly space velocity and oxygen to propylene molar ratio have been studied. A one-dimensional plug flow pseudo-homogeneous reactor model has been developed in order to interpret the 200 performed experiments. A set of kinetic parameters, minimizing the difference between the experimental results and those obtained by the model, is found by an optimization method.

**3. Design and validation of the HEXR**

The optimal operating conditions based on this new kinetic model have been determined in order to maximise acrolein yield. The yield is optimal for isothermal conditions, which is confirmed by the literature3. This isothermal behaviour can be achieved in an intensified HEXR4. The HEXR is designed by taking into account different constraints (process specifications, safety constraints, catalyst wash-coating constraints and maximal dimensions of the 3D printing machine) and then by calculating and studying different items:

* the number of channels required to convert the fixed mass flow rate of reactants,
* the fluid flow configuration (cross flow or co-current),
* the shape of fluid distributors and collectors,
* the temperature profile of the reactive and coolant sides.

Finally, after sizing the HEXR, some validations concerning safety aspects have been performed by CFD calculations. The influence of a potential thermal runaway is simulated in a section of the device to confirm the efficiency of the heat transfer. Besides, to evaluate the mechanical strength of the HEXR, a study is performed by using the temperature profile of the nominal case and by applying it to calculate the mechanical constraints on the structure. The same work is performed by considering a pressure gradient between both fluid sides.

**4. Conclusions**

An intensified mini-channel HEXR, presenting interesting performances, has been designed and manufactured by metal 3D printing. A complete simulation, coupled with the kinetic model, for a fraction of the device, as well as experiments on the manufactured unit, have yet to be done.

**References**

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