A 3D-1D model for the simulation of plant-scale chemical reactors

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ABSTRACT

A 3D-1D model has been developed to simulate the methane dehydroaromatization (MDA) process in plant-scale catalytic reactors. The 3D part of the model consists of CFD-DEM coupled simulations of some relevant volume elements (RVEs), while the 1D part is a low-order model bridging the solution between the RVEs; see the sketch in Figure 1a. The CFD-DEM model, implemented in the CFDEM®coupling software [1, 2], uses an immerse boundary method to resolve: 1) the flow around the catalytic structures, 2) the heat exchange between solid and fluid, 3) the MDA reaction at the fluid-catalyst interface. The CFD-DEM solution is scaled-up by the 1D model to allow the simulation of industrial-scale processes at acceptable computational cost. The effect of design parameters (e.g., catalyst geometry) and operating conditions (e.g., reactor operating temperature) on the methane conversion rate and pressure drop can be investigated using the proposed model and the main results will be presented.

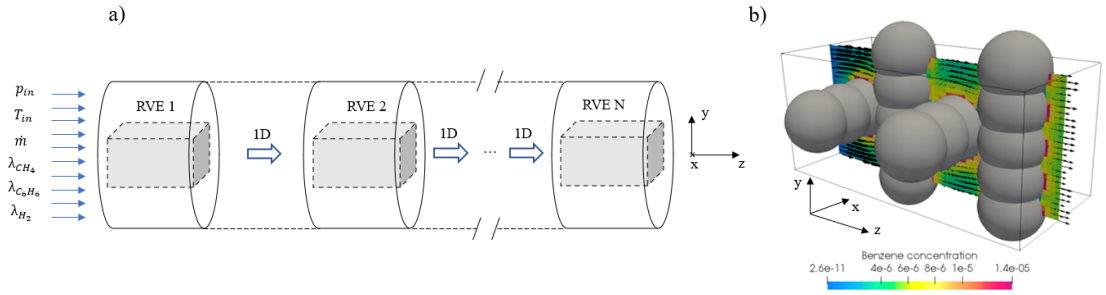

Figure 1: a) scheme the 3D-1D model. b) CFD-DEM simulation of an RVE. The catalyst is modelled using overlapping spheres (grey). The CFD slice is coloured with the benzene concentration.

REFERENCES

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Acknowledgement and disclaimer
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814548. This presentation reflects only the author's views and neither Agency nor the Commission are responsible for any use that may be made of the information contained therein.