Modeling of an industrial scale packed bed reactor for steam reforming applications

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INTRODUCTION: Methane Steam Reforming (MSR) is typically used to provide hydrogen required for the ammonia synthesis process. The modeling of an industrial scale, single tube, packed bed reactor for the MSR reactions can provide valuable information about the evolution both of gas species composition and of temperature profiles, along the axial and radial direction of the tube, as a function of catalyst packed bed features. This information can support the design and development of novel industrial reactors and catalyst particles.

COMPUTATIONAL METHODS and ASSUMPTIONS: Tightly coupled mass, energy, and momentum equations are set up using the physics interfaces of the *Chemical Reaction Engineering Module*. Brinkman equations, transport of concentrated species and the heat transfer in porous media physics are used to describe the velocity field, gas species concentration and temperature profiles along the reactor respectively, in a stationary state 2D-axialsymmetric simulation.

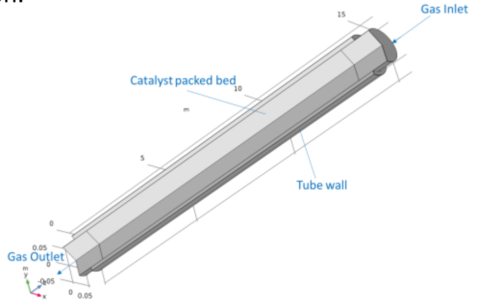

Figure 1. Single tube packed bed reactor geometry.

Turbulence in the flow field is taken into account applying the Algebraic yPlus RANS model with the Low Re wall treatment assumption. Thermodynamics module is used to consider the transport properties variation of the gas mixture along the tube due to the reactions. The chemistry of MSR is described implementing the kinetics model proposed by Xu and Froment [1]. Catalyst packed bed porosity (ε) is assumed both evenly distributed (ε = 0.4) and varying as a function of the tube radius and the catalyst particle shape and size ($\varepsilon = f(r, dp, di/dp)$ [2], [3]). The energy required to drive the endothermic reaction system is supplied through an external heat flux, provided across the tube wall (AISI 4340), in order to analyze the heat transfer by convection and conduction, even across the packed bed (Al_2O_3). Inlet gas composition and temperature are set at typical values of the industrial plants.

Variable	Value	Units
Total inlet molar flowrate	27.5	kmol/h
Inlet gas T, P	> 500, 60	°C, bar
Packed bed length	> 10	m
Tube internal diameter	9	cm
External duty	80	kW/m^2

Table 1. Main operating conditions.

RESULTS: MSR endothermicity affects the T profile along the axial direction of the tube: at the entrance of the catalytic bed reactions consume the heat provided (T ↑); concentration gradient of reagents progressively reduces (heat of reaction changes) and external heat better compensates the reactions' effect (T ↓). Radial gradients of T highlight the conduction effects in the catalyst bed.

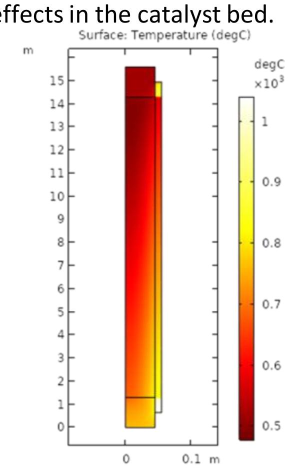

Figure 2. T profiles (ε = 0.4)

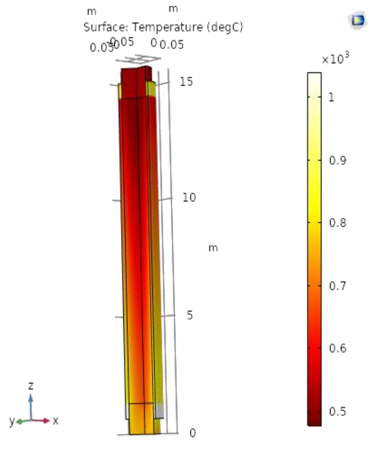

Figure 3. T profiles (ε = 0.4), 3D view.

CH4 slip in the outlet gas stream agrees with the equilibrium limited approach of the reaction kinetics model applied, at the outlet gas T, and fits well with industrial observations and with pressure drop values.

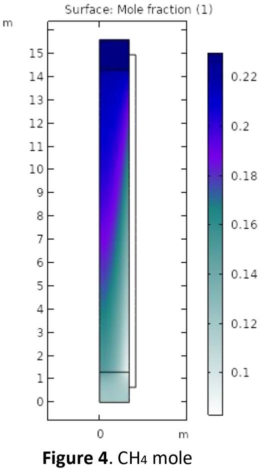

Figure 4. CH_4 mole fraction profile (ε = 0.4)

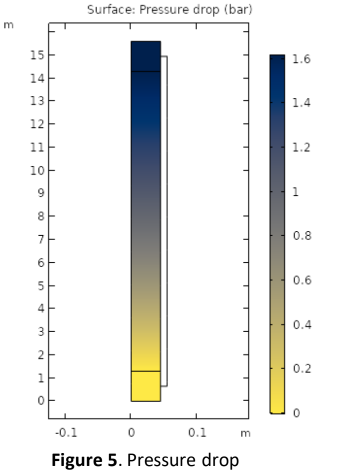

Figure 5. Pressure drop profile (ε = 0.4).

CONCLUSIONS: Results align closely with independent industrial evidence suggesting this model can be applied confidently to fast analysis/investigation of different catalyst bed packing, permeability and porosity features, as well as to different operating and reaction conditions. Such information enables faster screening and evaluation of new solutions for the MSR technology.

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