TOWARDS LARGE EDDY SIMULATIONS WITH DETAILED KINETICS

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Tubular reactors suspended in gas-fired furnaces are used extensively in the chemical and petrochemical industry for endothermic processes such as hydrocarbon pyrolysis and catalytic steam reforming. The efficiency of the process is mainly determined by the heat transfer rate of the combustion energy to the reacting process gas and can be improved by modifying the internal surface of the tube to obtain a variety of enhanced reactors (Van Cauwenberge et al., 2017). On the one hand, longitudinal and helicoidal fins increase the surface area and hence also the total heat flux to the reactor. On the other hand, internal structures are added to promote turbulence and secondary flow structures in the radial and azimuthal directions. Examples include the Mixing Element Radiant Tube (MERT) and variations. The major drawback of these enhanced reactors is the higher pressure drop, affecting both the product selectivities and yields. The optimization of these enhanced reactor tubes has been the subject of numerical studies (Schietekat et al., 2014). Many of these studies resort to Reynolds-averaged Navier-Stokes equations where values for the Reynolds stresses are obtained via closure models. As these models require tuning to experiments to be reliable, their predictive capabilities are limited. Turbulence resolving techniques such as large eddy simulations (LES) and direct numerical simulations (DNS) limit or avoid the use of closure models by resolving the effect of turbulence explicitly: turbulent eddies are captured by defining a sufficiently small time step and sufficiently high mesh resolution. Using these eddy resolving techniques allows to capture the important interplay between turbulence and the rate of chemical reactions. LES simulations of enhanced tubular reactors implementing a detailed chemical reaction network for pyrolysis have been carried out in this work. They provide detailed insight in the time and length scales of the additional turbulent structures introduced in the fluid by the enhanced reactor geometry and allow to reliably predict the change in product yields.

Figure 1: Inner wall temperature [K] in a section of a ribbed tube during steam cracking of ethane


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