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Dynamic simulation of fouling in steam cracking reactors using CFD

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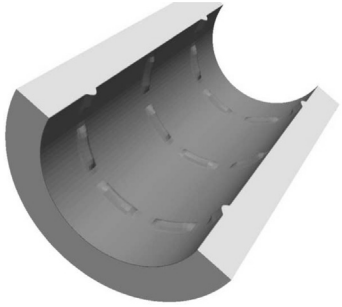
HIGHLIGHTS

- An algorithm to simulate coke formation in 3D steam cracking reactors was developed.
- Taking into account coke layer growth is needed to evaluate a reactor's run length.
- Three Millisecond propane crackers were simulated over the first days of their run.
- The longest run length was found for the ribbed reactor design.

GRAPHICAL ABSTRACT



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ABSTRACT

Recently computational fluid dynamics (CFD) has been successfully applied for the evaluation of the start-of-run performance of three-dimensional (3D) coil geometries in steam cracking reactors. However, determining the full economic potential of a coil involves tracking its performance throughout the run and not only at start-of-run. Therefore in this work a novel method has been developed that allows to assess the most debated characteristic of these 3D coil geometries, i.e. the potential extension of the run length in combination with the evolution of the product yields during the time on stream. An algorithm based on dynamic mesh generation is presented for simulating coke formation in 3D steam cracking reactor geometries, tracking the apparent geometry deformation caused by the growing coke layer. As a proof-of-concept, a Millisecond propane cracker is simulated over the first days of its run length, and this for three different coil designs: a bare tube, a finned tube and a continuously ribbed reactor design. Our simulations show that the ribbed reactors overall outperform the others although in these enhanced tubular geometries the growth of the coke layer is far from uniform. Because of this, the reactor geometry will change over time, which will in turn influence the fluid dynamics, product yields and successive coke formation substantially.

1. Introduction

Steam cracking of hydrocarbons is the predominant industrial process for the production of many commercially important base chemicals such as light olefins (ethene, propene, butadiene) and aromatics (benzene, toluene, xylenes). These base chemicals are the key building blocks for large-volume polymers and other high-value chemicals. Steam cracking is one of the most energy-intensive processes in the chemical industry, representing approximately 8% of the sector's primary energy consumption [1]. A major factor for the process energy efficiency is the formation of coke on the inner wall of the tubular cracking reactors. This growing carbonaceous layer has two negative effects. First of all, the reactor pressure drop increases as the cross-sectional flow area decreases, resulting in a loss of selectivity to ethylene, the process' main product [2]. Secondly, the highly insulating coke layer blocks the heat transfer from the furnace to the process gas. To maintain the same

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Nomenclature

Roman

J	Diffusion flux [kg m^{-2} s^{-1}]
R	Rate of formation [kg m^{-3} s^{-1}]
S_h	Chemical enthalpy source term [J m^{-3} s^{-1}]
Y	Mass fraction [–]
n_k	Total number of species [–]
q	Sensible enthalpy flux [J m^{-2} s^{-1}]
u	Velocity [m s^{-1}]
x	Position [m]
h	Specific enthalpy [J kg^{-1}]
Pr	Prandtl number: Pr = $\mu c_p/\lambda$ [–]
Sc	Schmidt number: $Sc = \mu/\rho D$ [–]
T	Temperature [K]
k	Turbulent kinetic energy [m^2 s^{-2}]
p	Pressure [Pa]

Greek

λ	Thermal conductivity [W m^{-1} K^{-1}]
μ	Dynamic viscosity [kg m^{-1} s^{-1}]
ρ	Density [kg m^{-3}]
φ	Arbitrary transported variable
τ	Stress tensor [Pa]

Sub- and superscripts

i	In the i-th direction
j	In the j-th direction
k	Of the k-th species
f	Of the fluid
s	Of the solid
t	Turbulent

Abbreviations

CFD	Computational Fluid Dynamics
COT	Coil Outlet Temperature [K]
COP	Coil Outlet Pressure [Pa]
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
TMT	Tube Metal skin Temperature [K]

cracking severity, the heat input is increased to counteract the increased heat transfer resistance, leading to higher tube metal temperatures (TMT) and still higher coking rates. Eventually, either due to an excessive pressure drop over the reactor or due to metallurgical constraints of the reactor tube alloy, production needs to be halted to decoke the reactor. These periodic production interruptions have a clear negative effect on the process economics. Furthermore, the reactor lifetime deteriorates with successive coking-decoking cycles because of tube corrosion, carburization and erosion [3–6].

In response to this economic and environmental drawback, several technologies to reduce coke formation have been investigated [7–10]. One such technology is the use of three-dimensional (3D) reactor geometries to enhance radial mixing and facilitate heat transfer to the process gas. As coke deposition is a chemical process, the reduced tube metal temperatures have been shown to result in lower coking rates and longer furnace run lengths [11]. Previously, computational fluid dynamics (CFD) has been applied to evaluate the start-of-run performance of these 3D reactor geometries and to assess their effect on pressure drop, coking rates and product yields [11,12]. However, as the most attractive characteristic of the enhanced reactor designs is the extension of the furnace run length, not only start-of-run performance should be evaluated to determine the potential of a 3D coil but also its performance throughout the run, i.e., as function of the time-on-stream. In the case of 3D tubular geometries or reactors with a strongly non-uniform heat flux profile (e.g. due to shadow effects), the growth of the coke layer will generally not be uniform. Because of this, the apparent reactor geometry will change in time, which will in turn influence the fluid dynamics, product yields and successive coke formation. In order to obtain an accurate prediction of a reactor's run length, all these phenomena need to be accounted for and hence the coke layer growth needs to be incorporated in the CFD simulations. The methodology presented in this work allows to track the apparent deformation of the flow domain caused by the growing coke layer, in this way making it possible to perform run length simulations of (industrial-scale) steam cracking reactors. The method is based on dynamic mesh generation, and can be applied for a variety of frequently encountered reactor designs. As a proof-of-concept, the method is used to simulate a Millisecond propane cracker over the first days of its run, and this for a bare tube, a longitudinally finned tube and a continuously ribbed tube design.

2. CFD model

2.1. Governing equations

The steady-state governing equations for a compressible, reactive, single-phase fluid flow are the following:

$$\frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} \tag{2}$$

$$\frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial q_i}{\partial x_i} + S_h \tag{3}$$

$$\frac{\partial \rho Y_k u_i}{\partial x_i} = -\frac{\partial J_{k,i}}{\partial x_i} + R_k \quad (\forall k = 1, n_k - 1) \tag{4}$$

To be able to explicitly account for the heat transfer from the metal reactor outer wall to the process gas (conjugate heat transfer), the Laplace equations for thermal conduction in the coke layer and metal tube wall surrounding the process gas are solved simultaneously with the governing equations for the fluid flow.

$$\nabla \cdot (\lambda_s \nabla T) = 0 \tag{5}$$

In the above equations, τ_{ij} is the viscous shear stress tensor, which is evaluated using the Boussinesq eddy viscosity concept. The sensible enthalpy flux q_i and the diffusion flux $J_{k,i}$ are both modeled using an eddy diffusivity approach:

$$\tau_{ij} = (\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3} k \delta_{ij} \tag{6}$$

$$q_i = c_p \left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t}\right) \frac{\partial T}{\partial x_i} \tag{7}$$

$$J_{k,i} = \left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right) \frac{\partial Y_k}{\partial x_i} \tag{8}$$