# Prediction of coke formation in oil-refinery equipments

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**Abstract**

Coke formation is a process that can seriously affect the performance of oil-refinery equipments. A numerical prediction of coke formation due to thermal cracking and oxidation of vacuum residue is presented in the paper. Relevant models have been implemented into the commercial CFD code by means of user subroutines technique. Subsequent tests revealed that the numerical results fit experimental data obtained from literature. Presented method can be employed for processes optimization.

## 1 Introduction

Coke is an insoluble fraction of asphalt, sedimenting due to thermal cracking and oxidation processses. Oxidation reaction within vacuum residues is exothermal, thus creates local high temperature domains. This is the reason to asphalt overheating that results in coke deposition. Its production can badly affect oil-rafinery equipments, leading to momentum losses or heat transfer rate decrease thus forcing more frequent servicing periods. Hence importance of numerical prediction for better and cheaper process optimization.

## 2 Model details and numerical computations

The model employed in the present study bases directly on the propositions by Souza et al. [1] and Yutai [2]. The model is built on the preassumption that the flow is steady-state and laminar one. We assume also that asphalt can be treated as newtonian fluid and its composition consists of seven pseudo-components as in original paper [1]. Coke formation model was implemented into CFD commercial code [3] with user subroutine technique. The basic set of balance equations has been extended to cope with additional

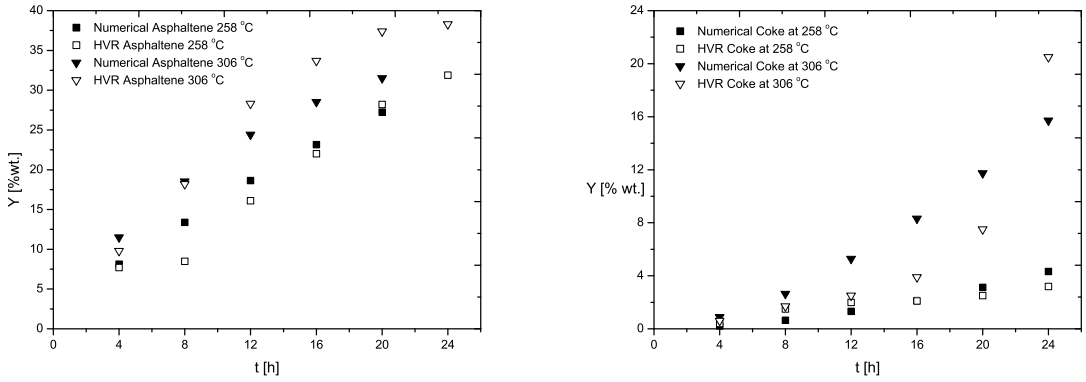
transport equations for particular pseudocomponent. It can be written as in [4]:

$$\frac{\partial}{\partial t}\begin{Bmatrix}\rho\\ \rho\vec{v}\\ \rho e\\ \rho Y_1\\ .\\ .\\ \rho Y_n\end{Bmatrix} + \mathrm{div}\begin{Bmatrix}\rho\vec{v}\\ \rho\vec{v}\otimes\vec{v}\\ \rho e\vec{v}\\ \rho Y_1\vec{v}\\ .\\ .\\ \rho Y_n\vec{v}\end{Bmatrix} + \mathrm{div}\begin{Bmatrix}0\\ p\overleftrightarrow{I}\\ p\vec{v}\\ 0\\ .\\ .\\ 0\end{Bmatrix} = \mathrm{div}\begin{Bmatrix}0\\ \overleftrightarrow{\tau}_c\\ \overleftrightarrow{\tau}_c\vec{v}+\vec{q}_c\\ \vec{J}_{Y_1}\\ .\\ .\\ \vec{J}_{Y_n}\end{Bmatrix} + \begin{Bmatrix}0\\ \rho\vec{b}\\ \rho S_e\\ \rho S_{Y_1}\\ .\\ .\\ \rho S_{Y_n}\end{Bmatrix} \quad , \quad (1)$$

where: $Y_k$ - mass fraction of single pseudocomponent, with k ranging from 1 to n.

Way of model implementation is similar to given by Souza et. al. [1]. Changes of mass fraction are modeled as sources $S_k$, which are rate constant functions. Rate constants and boundary conditions were assumed to be same as in Yutai [2].

Implemented model has been verified by means of experimental data presented in an original paper [2]. It's shown that numerical prediction of coke formation well corresponds to experimental data thus confirms model implementaion.




a) b)

Figure 1: Pseudocomponent contents changes with reaction time - mass fraction of a) coke and b) asphaltens. Filled points reffer to numerical data.

# 3 Summary

In the paper brief introduction into issue has been presented. Fundamentals of the model and its implementation has been described. In the conclusion it has been shown that there is strong correlation between numerical and experimental data, indicating model by Souza et al. [1] description to be correct or at least very well corresponding to phenomenon nature.

# References


[1] B.A. Souza, E.M. Matos, R. Guirardello and J.R. Nunhez, Predicting coke formation due to thermal cracking inside tubes of petrochemical fired heaters using fast CFD formulation, *J. Petroleum Sci. Eng.* **51** (2006) pp. 138-148

[2] Q. Yutai, Investigation of serial reaction kinetics and changes of group compositions of vacuum residues in continuous oxidation, *Fuel* **79** (2000) pp. 1815-1821

[3] *FLUENT User's Guide*, Fluent Inc., Lebanon, USA, 1997–2002,

[4] J. Badur, *Numerical modelling of sustainable combustion in gas turbines*, IFFM Publishers, Gdańsk, 2003