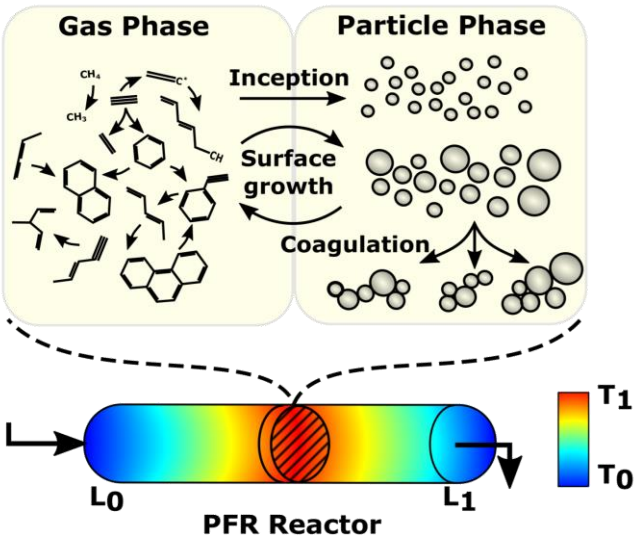
User Story

Modelling study of Carbon Black (CB) formation at different operating conditions



THE CHALLENGE

To predict the evolution of CB particles along the PFR length at various operating conditions.

THE SOLUTION

- Use CMCL's *k*inetics software to simulate the CB formation and dynamics in a plug flow reactor (PFR)
- Apply the 1D and 2D population balance soot models solved using method of moments (MOM) and sectional method (SECT)
- Detailed gas phase chemical mechanism from literature [2].

THE RESULTS

Evolution of the coupled gas-particle phases along the reactor length:

- Chemical species concentrations profiles
- Particle volume fractions
- Average particle size and/or particle size distribution
- Average number of primaries per aggregate.

OVERVIEW

Carbon Black (CB) is a nano-sized material that is often regarded as a pure form of soot. Many different CB manufacturing methods exist having an incomplete combustion or thermal decomposition of gaseous or liquid hydrocarbons at their cores. CB particles find applications in e.g. tyre, rubber, plastic or coating industries where specific particle size distribution (PSD), surface area or even morphology of produced particles are required.

This use-case describes a modelling study of CB formation in PFR reactors. The resulting population balance models (1D and 2D) are solved using method of moments (MOM) and method of sections (SECT) to predict properties such as average particle size and number of primaries per aggregate, aggregate PSD and concentration profiles of selected gaseous species. All calculations were performed with the *k*inetics™ software.

CASE DESCRIPTION

Selected experimental scenarios have been taken from the Naseri and Thomson's work [1], where CB aggregates are formed in a heated tubular reactors via thermal pyrolysis of:

I. 1.0% CH_4, 0.75% O_2 and 98.25% N_2 using five experimental temperature profiles with their nominal peaks (T_1) within the 1073-1873 K range, reactor length L_1 = 2 m and flow rate of 5 Nl/min. Experimental data for this case originally came from Skjøth-Rasmussen's work [3].

II. 1.0% C_2H_4 and 99.0% N_2 using an experimental temperature profile with a nominal peak temperature T_1 = 1700 K, reactor length L_1 = 0.64 m and flow rate of 2 Nl/min. Experimental data for this case originally came from Dewa's work [4]

CMCL's MOM and SECT methods with PYRENE as an inception species and CRECK[1] chemical mechanism have been used in all simulated cases to account for the coupled gas-particle phase evolution.

[1] Downloaded from the supplementary section of [2]

1. A. Naseri, M. J. Thomson, *Combust. Flame, 314-326, 2007*
2. E. Ranzi, A. Frassoldati et al., *Prog. Energy Combust. Sci.*, *468-501, 2012*

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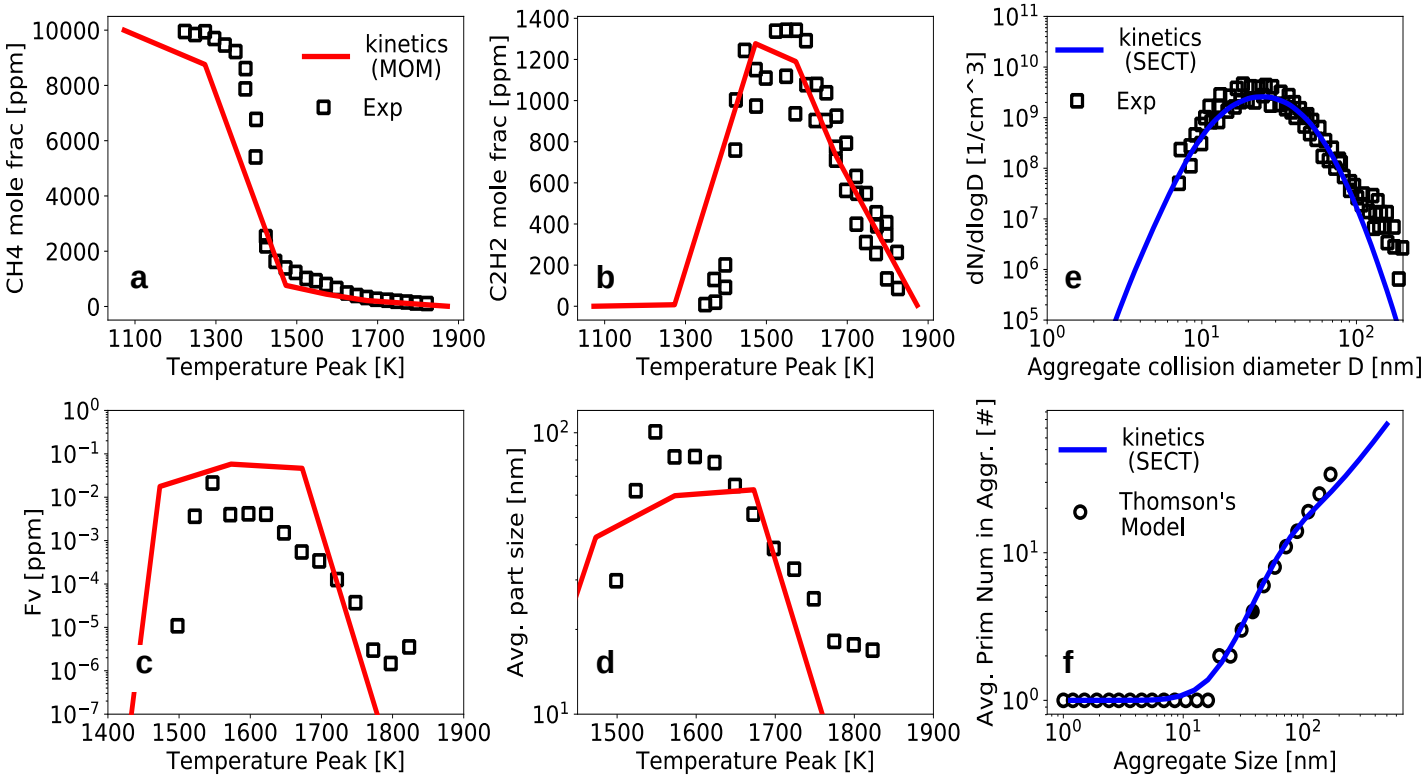

Figure 1: Gas and particle phase evolution in the experimental case I (plots a-d) and in the experimental case II (plots e-f). Solid lines represent modelling results in *k*inetics™ with the method of moments (red) and a sectional method (blue). Experimental and modelling data are taken from literature [1] and are represented by hollow square and circle markers respectively.

RESULTS

Main simulation results are depicted on Fig.1. Plots a-d show results for the experimental case I that include concentration of selected chemical species, particle volume fractions and particle average sizes as a function of nominal peak temperature. Plots e-f show results for the experimental case II that include particle size distribution and average number of primaries in aggregates.

From the case I results, it can be seen that the evolution of selected gas-phase species (CH_4 and C_2H_2) compares well against the experimental data (plots a-b). Good greement is also obtained for other (*not plotted*) hydrocarbon species. The particle volume fractions, Fv and particle average sizes (plots c,d) are also well reproduced (within the range of experimental values) given the fact that the method of moments resolves only average particle quantities.

For the case II results, it can be seen that the sectional method reproduces the experimental particle size distribution well (plot e). In addition to that, the calculated average number of primaries per aggregate (plot f) matches closely with Naseri and Thomson's modelling results [1], which in turn compare favourably against experimental SEM images from Dewa et al. [4].

APPLICATION AREAS

- Carbon Black modelling

PRODUCTS USED

- *k*inetics™

3. M. S. Skjøth-Rasmussen, P. Glarborg et al., *Combust. Flame*, 91-128, 2004

4. K. Dewa, K. Ono et al., *Combust. Flame*, 115-121, 2016