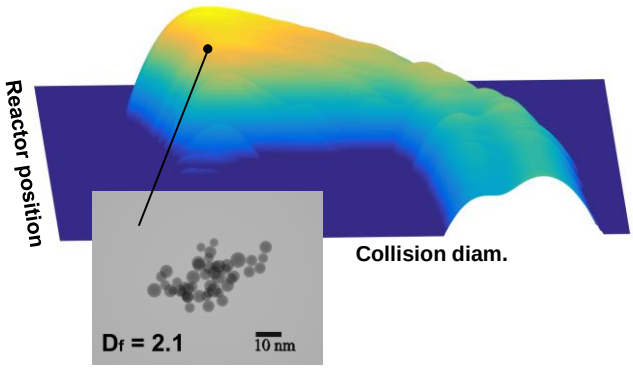
User Story

Morphology and Fractal dimension of carbon black aggregates – a detailed stochastic approach in *kinetics*™



OVERVIEW

Carbon Black (CB) is a nano-sized material of the form of colloidal particles that are produced by incomplete combustion or thermal decomposition of gaseous or liquid hydrocarbons. Some of the CB applications are tyre, rubber, plastic or coating industries where specific particle size distribution (PSD), surface area or even morphology of produced particles are required. This example describes how morphology of CB particles, in form of 3D structures of CB aggregates and their fractal dimensions, can be calculated using kinetics™ toolkit.

THE CHALLENGE

To predict the evolution of fractal dimension of carbon black aggregates along the length of the reactor.

THE SOLUTION

- Description of the carbon black system in terms of particle processes (a detailed Population Balance Model) and gas-phase processes (a chemical kinetic model).
- Coupling the two models together and solving for given conditions in a Plug Flow Reactor (PFR).
- Sampling of the representative aggregates along the reactor and resolving their shapes via ballistic aggregation.
- Calculation of the mass/volume-fractal dimensions of the sampled aggregates.

THE RESULTS

- Evolution of Particle Size Distribution (PSD) of carbon black aggregates.
- 3D structures of the selected aggregates sampled at different positions along the reactor.
- Fractal dimension of the sampled aggregates.

CASE DESCRIPTION

An experimental scenario has been selected from the literature [1], where CB aggregates are formed in a heated tubular reactor via thermal pyrolysis of various mixtures of benzene and acetylene in nitrogen. The selected scenario is schematically shown on Fig.1.

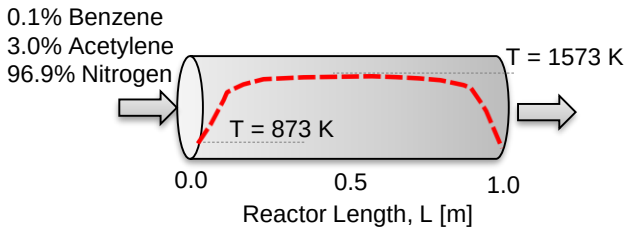


Figure 1: Process conditions selected from the literature [1]

The Carbon Black system model formulated within kinetics™ comprises a detailed gas-phase chemical kinetic model and a detailed particle-phase stochastic population balance model.

MORPHOLOGY AND FRACTAL DIMENSION PREDICTION

Upon successful solution of the CB system, detailed information about a number of representative aggregates (number and size of primaries, chemical composition, collision diameter etc..), selected at specified reactor's positions is then used to create 3D structures (in the form of a TEM-like image) of the sampled aggregates via ballistic aggregation procedure.

[1] K. Ono, M. Yanaka, Y. Saito, H. Aoki, O. Fukuda, T. Aoki and T. Yamaguchi, *Chem. Eng. J., 215-216, 2013*

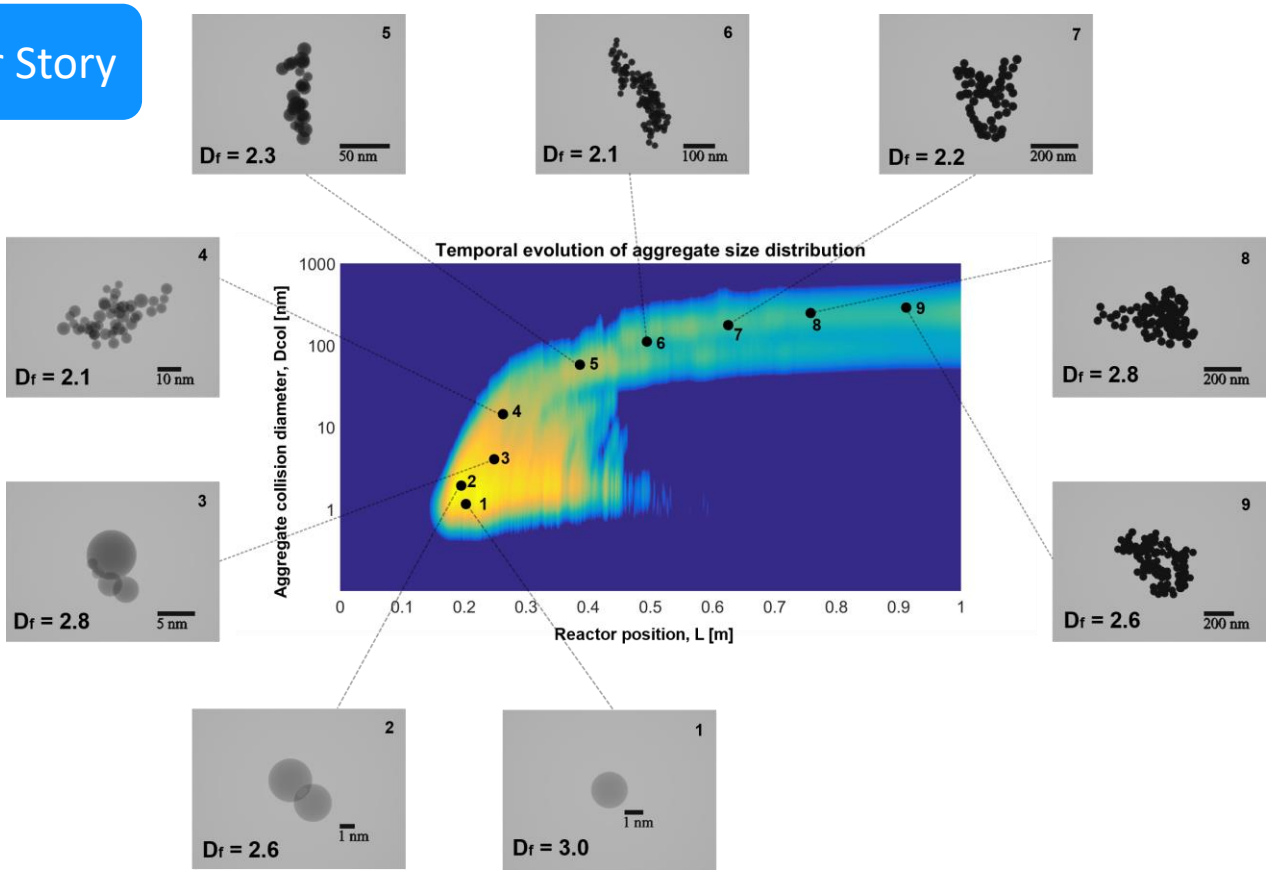


Figure 2: Evolution of Carbon Black aggregate particle size distribution (PSD) along the reactor. Colormap encodes normalized particle concentration, dN/dlogD [#/cm^3], y axis represents average aggregate collision diameter and x axis shows position on the reactor. Structures of selected aggregates in form of TEM images are also shown along with their calculated fractal dimensions.

RESULTS

Main simulation results in Fig.2 depict the evolution of particle size distribution of carbon black aggregates along the reactor together with calculated morphologies and fractal dimensions of selected aggregates. Colormap encodes normalized particle concentration, *dN/dlogD* [#/cm^3], y axis represents average aggregate collision diameter, D_{col} *[nm]*, and x axis shows position on the reactor, *L [m]*.

It can be seen that the CB particles start to form around 0.2m from the reactor's inlet, where the temperature rises to around 1530 K. Initially, the aggregates formed contain small number of primaries and are of spherical shape (1-3), hence their fractal dimension is close to 3.0. Further into the reactor, the aggregates start to coagulate and grow via surface reactions. The interplay between these two processes together with constant inception of small primaries leads to the formation of more complex structures (4-7). At the reactor's outlet, the sampled aggregates (8-9) are close to the spherical shape.

Comparing sampled aggregates with the experimental TEM image from the literature [1] shows that there is an agreement in terms of morphology and aggregate sizes.

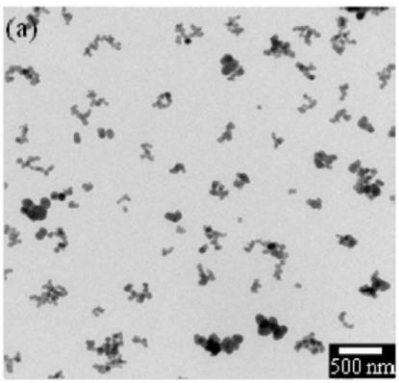


Figure 3: Experimental TEM data from Ono et al. [1]

APPLICATION AREAS

- Carbon Black modelling

PRODUCTS USED

- *k*inetics™