User Story

Hot-wall reactor for the gas-phase synthesis of inorganic nanomaterials

A hot-wall reactor model from kinetics™ applied to the gas-phase synthesis of silicon from silane.

THE CHALLENGE

To accurately and rapidly simulate the gas-phase synthesis of inorganic nanomaterials in a hot-wall reactor, accounting for the interaction between particle and gas phase.

THE SOLUTION

- A detailed mechanism describing gas-phase chemistry, particle inception, surface reactions and particle coagulation
- The computationally non-intensive method of moments for the solution of the population balance model

THE RESULTS

- Fast simulation of detailed chemical kinetic models for a growing family of inorganic nanoparticle synthesis processes in *k*inetics™
- Particle process rates and nanoparticle aggregates elemental composition simulated by the model
- Ability to evaluate particle properties including number of particles and particle average diameter, as well as gas-phase composition, system temperature and pressure, and other relevant physical quantities of the hot-wall reactor

OVERVIEW

A new reactor model has been added to CMCL Innovations' proprietary software *k*inetics™. It will be used for the simulation and optimisation of hot-wall processes for the synthesis of inorganic nanomaterials.

The reactor was initially based on the hot-wall reactor design used at the University of Duisburg-Essen (see Figure 1) and has been developed as one of the deliverables of the ongoing NanoDome project (Horizon 2020) (http://www.nanodome.eu/) aimed at developing a robust model-based approach for the prediction of nanomaterial structures in commercially relevant gas-phase synthesis processes.

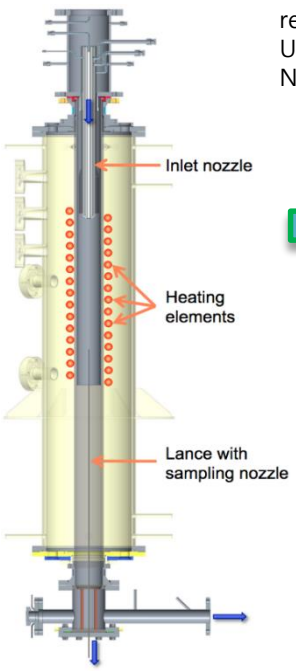

Figure 1: Schematic of hot-wall reactor (provided by the University of Duisburg-Essen – Nanoparticle Synthesis group)

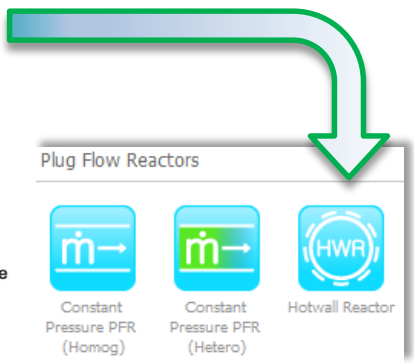

Figure 2: Screenshot from the library of reactors in *k*inetics™.

The model is based on a PFR (Plug Flow Reactor) design (Figure 2). The axial temperature profile along the reactor can be either evaluated from energy equations or imposed by the user. A number of nanoparticle synthesis mechanisms have been used and tested in the hot-wall reactor model. The mechanism for the synthesis of silicon from silane is currently provided with the *k*inetics™' installer.

NanoDome project has received funding form the European Union's *Horizon 2020 Research and Innovation Programme*, under Grant Agreement n° 646121

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RESULTS

The hot-wall reactor developed in *k*inetics™ has been used to simulate a number of systems, including silicon from silane and metallurgical silicon, SiO_2 from TEOS, TiO_2 from $TiCl_4$, and TiO_2 from TTIP.

Available experimental results for the synthesis of silicon from silane were used here to validate the model developed in *k*inetics™[1]. Some of the results from the validation study are presented in Figure 3. These results were obtained for mixtures of SiH_4-Ar at different operating conditions.

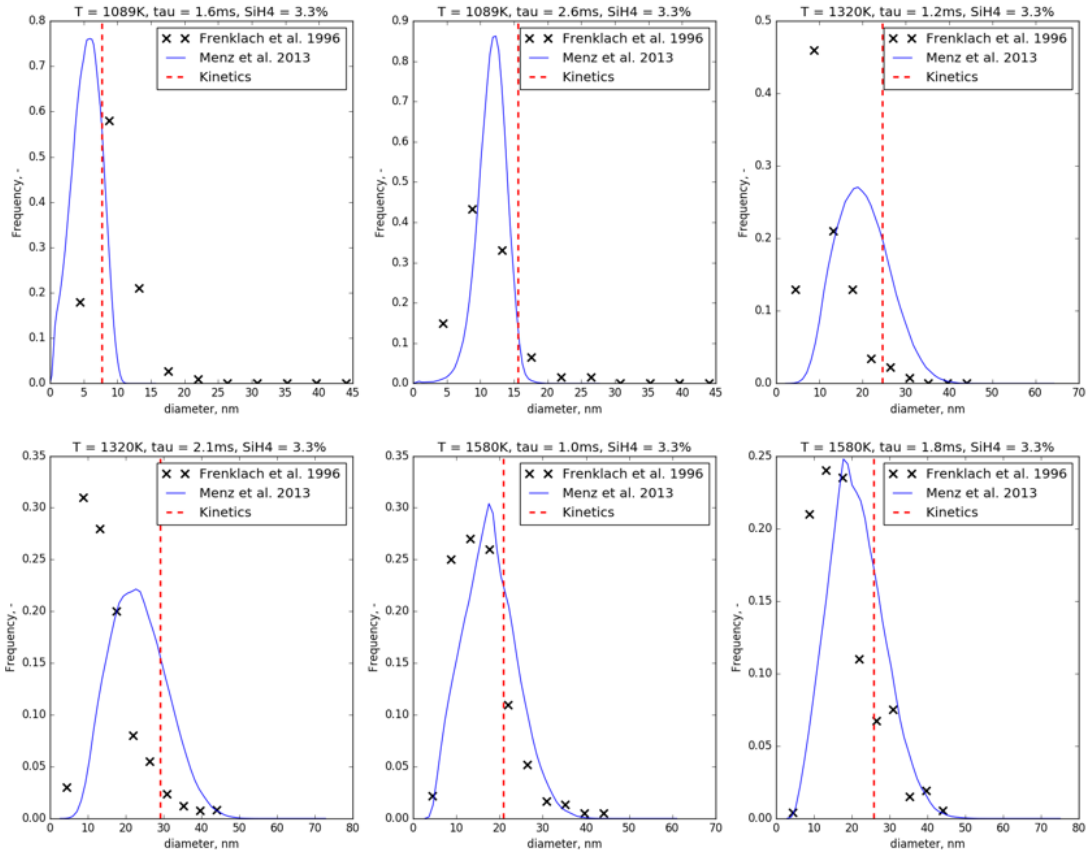

Figure 3: Average diameter of silicon nanoparticles simulated using *k*inetics™' hot-wall reactor and comparison with experimental data from Frenklach et al. (1996)[1] and simulation results from the Menz and Kraft (2013)[2] model, used as benchmark for the model.

APPLICATION AREAS

- Gas-phase synthesis of inorganic nanoparticles in hot-wall reactors
- Reduction of finite rate kinetic schemes to be used in the reactor model and third-party 3D toolkits

PRODUCTS USED

- *k*inetics™
- Hierarchy of chemical kinetic models, from detailed to skeletal (mechanism for the gas-phase synthesis of silicon from silane currently provided with *k*inetics™)

[1] M. Frenklach, L. Ting, H. Wang, M.J. Rabinowitz, Israel Journal of Chemistry 36 (3) (1996) 293–303.
[2] W. J. Menz and M. Kraft. *Combustion and Flame*, 160(5): 947-958, 2013.

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