User Story

A reactor network approach in *k*inetics™ to model the gas-phase synthesis of nanoparticles in DC plasma reactors

THE CHALLENGE

To predict the characteristics of nanomaterials produced in DC (Direct Current) plasma reactors using a fast-response toolkit able to accurately capture relevant properties of both particle and gas phases.

THE SOLUTION

- Implementation of the computationally non-intensive method of moments to solve the population balance for the particle phase
- Formulation of a hierarchy of detailed chemical kinetic mechanisms for the synthesis processes
- Modelling via reactor networks to accurately capture the details of each zone of the plasma reactor

THE RESULTS

- Rapid and accurate simulation of the gas phase synthesis of selected nanomaterials in DC plasma reactors within *k*inetics™
- Prediction of particle process rates, nanoparticle aggregates elemental composition and relevant nanoparticle properties, including number of particles and particle average diameter
- Evaluation of gas-phase composition, system temperature and pressure, and other relevant physical quantities in the plasma reactor
- Modelling of plasma source, heat transfer and turbulent mixing in the reactor

OVERVIEW

A model for the simulation of DC plasma reactors is available in CMCL's proprietary software *k*inetics™. The model is based on a design proposed by the University of Bologna (see Figure 1) to describe an industrial-scale DC plasma reactor used at Umicore for the production of ZnO nanoparticles. The model has been developed as part of the NanoDome project (http://www.nanodome.eu/), sponsored by the EU under the Horizon 2020 programme.

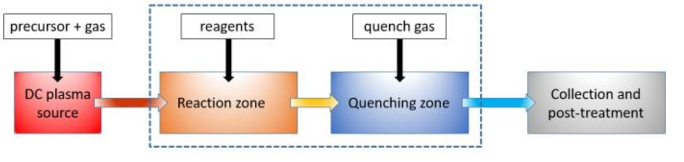

Figure 1: Schematic of a DC plasma reactor proposed by the University of Bologna and based on an original design from Umicore.

The model was formulated within *k*inetics™ as two reactors in series, one simulating the reaction zone and the other the quenching zone, as shown in Figure 2. This modelling strategy utilises the reactor network capabilities of *k*inetics™.

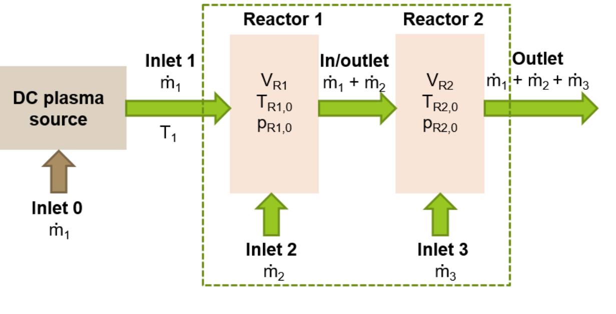

Figure 2: Representation of a plasma reactor as a reactor network for implementation in *k*inetics™.

NANODOME

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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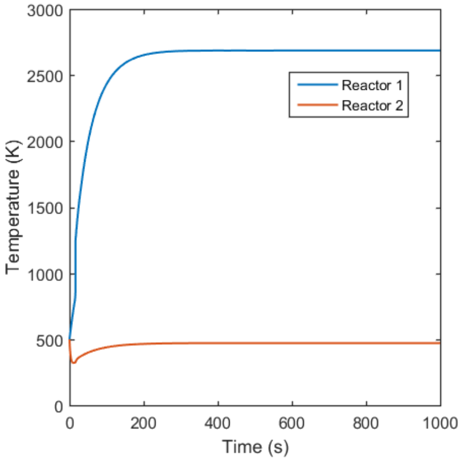

Figure 3: Temperature evolution in a DC plasma reactor as simulated in *k*inetics™ (reactor 1: reaction zone; reactor 2: quenching zone).

The particle population balance is solved using the method of moment with interpolative closure (MoMIC).

RESULTS

The plasma reactor model in *k*inetics™ can currently be used to simulate a number of nanomaterial synthesis processes, including ZnO from ZnO micro-powder and silicon from metallurgical silicon. Other nanomaterial synthesis processes can be added if suitable kinetic mechanisms are available.

APPLICATION AREAS

- Simulation of gas and particle phase evolution in DC plasma reactors during the gas-phase synthesis of inorganic nanomaterials
- Study different reactor configurations to simulate the plasma process using the reactor network capabilities

PRODUCTS USED

- *k*inetics™
- Hierarchy of chemical kinetic models, from detailed to skeletal (models for the gas-phase synthesis of ZnO from ZnO micro-powder are currently provided with *k*inetics™)

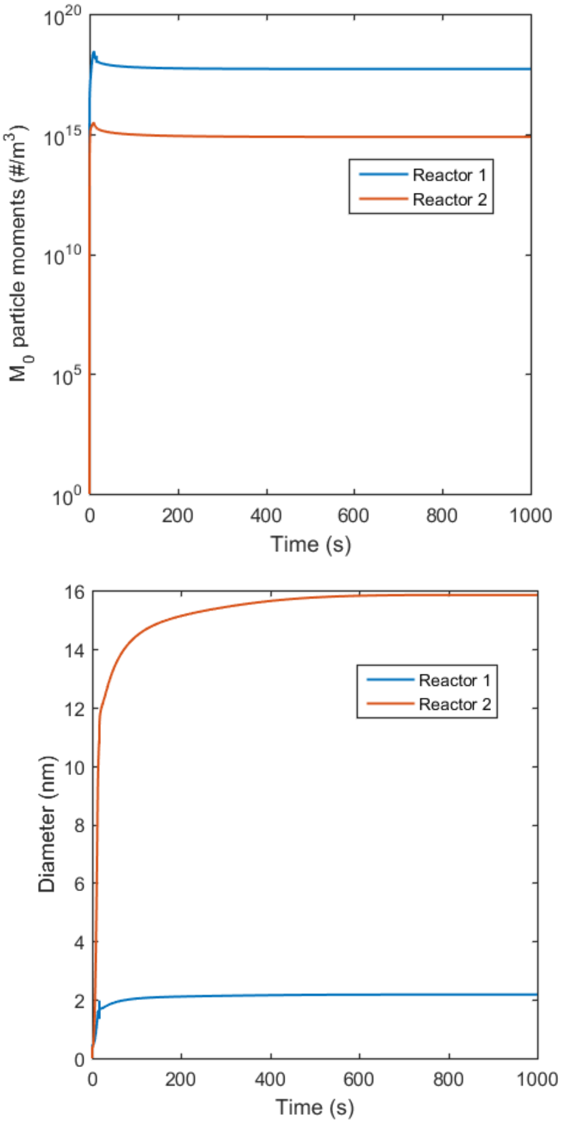

Figure 4: Total number of ZnO particle (zeroth moment of the distribution) and average particle diameter in a DC plasma reactor as simulated in *k*inetics™ (reactor 1: reaction zone; reactor 2: quenching zone).

Results from the simulation of the ZnO synthesis process are presented in Figures 3 and 4. Constant volume homogeneous reactors were used to simulate the two zones of the plasma reactor. Condensation due to sudden cooling (Figure 3) during quenching causes the number of particles to reduce and their diameter to increase in the quenching zone (Figure 4).

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