Modelling of fullerene production cell

Katarina Mramor[1], Božidar Šarler [2]

1: Laboratory for Advanced Materials Systems, Center of excellence for Biosensors, Instrumentation and Process Control - COBIK, Velika pot 22, SI-5250 Solkan
2: Laboratory for Multiphase Processes, University of Nova Gorica

One of the most effective techniques to synthesize fullerens and nanotubes is to vaporise graphite based electrodes in a low pressure inert gas atmosphere. To comprehend the process of the fullerene formation, reduce the cost of the material and improve the efficiency of the production technique, a better understanding of the nucleation and growth of carbon clusters is necessary. The nucleation and growth mechanisms are approximated by chemical kinetics model that is strongly coupled with a mathematical model which describes the physical behaviour of non-equilibrium plasma.
The growth mechanism is proposed for a two dimensional axial symmetric reactor chamber. The reduced chemical kinetics model applied for this purpose consists of 18 chemical reactions and 7 reacting carbon species for fullerene formation and additional 50 reactions and 20 species for nanotube formation. The interactions between species in the model are described by Arrhenius temperature relation, rate of progress and reaction rate equations. The equations of chemical kinetics model are strongly coupled with the governing equations of the mathematical model (continuity equation, momentum conservation equation, species conservation equation and energy conservation equation).
Chemical kinetics model is used to explain the formation of carbon clusters and the mathematical model describes the dynamics of species in fullerene production cell. The proposed chemical kinetics model accounts for the concentration and mass fraction of reacting species, whereas the mathematical model explains the behaviour of mass, velocity and temperature as well as the distribution of species in the production cell.
The equations of suggested chemical kinetics model are solved with Euler's method and the governing equations of the suggested mathematical model are solved with a Local Radial Basis Functions Collocation Method (LRBFCM), structured on multiquadrics radial basis functions with five-noded influence domains and explicit time stepping.

Here, a numerical implementation of chemical kinetics model for fullerene formation is presented and tested for 18 reactions and 7 carbon species.
Ensuing is the implementation of the mathematical model with the existing chemical kinetics model.

References:

J-F. Bilodeau, J. Pousse, A. Gleizes. (1998) A mathematical model of the carbon arc reactor for fullerene synthesis. Plasma Chem. and Plasma Process. 18, 285-303

I. Hinkov, S. Farhat, C. D. Scott. (2005) Influence of the gas pressure on single-wall carbon nanotube formation. Carbon 43, 2453-2462

A.V. Krestinin, A.P. Moravsky. (1998) Mechanism of fullerene synthesis in the arc reactor. Chem. Phys. Lett. 286, 479-484

A.V. Krestinin, A.P. Moravsky. (1999) Kinetics of fullerene C_{60} and C_{70} formation in a reactor with graphite rods evaporated in electric arc. Chem. Phys. Reports 18, 515-532

C. D. Scott. (2004) Chemical Models for Simulating Single-Walled Nanotube Production in Arc Vaporisation and Laser Ablation Processes J. Nanosci. Nanotechnol. 4, 368-376

B. Šarler and R. Vertnik. Meshfree explicit local radial basis function collocation method for diffusion problems. Comp.& Math. with App., 51:1269-1282, 2006.

G. Kosec and B. Šarler. Solution of thermo-fluid problems by collocation with local pressure correction. Int. J. Num. Meth. Heat & Fluid Flow, 18:868-882, 2008.

Figure 1: Carbon mass fraction.