Numerical Modelling of Fullerene Production by the Arc-Discharge Method - A Meshless Approach

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This paper describes a numerical model for simulation of the arc - discharge reactor for production of fullerenes. Fullerenes are carbon molecules in which carbon atoms are arranged in cylindrical, spherical or ellipsoid structure.

The arc-discharge apparatus consists of a cooled reactor chamber in which two electrodes; cathode and anode, are placed a small distance apart. Plasma which is created between the electrodes, ensures the anode evaporation. Fullerenes and nanotubes are formed from supercooled and supersaturated vapour, the result of plasma quench at the edges.

The physical model consists of the equations for conservation of mass, energy, momentum and species (carbon atoms, small carbon molecules from C_2 to C_{10}, carbon cycles and polycycles including molecules with 11 to 31 carbon atoms, fullerenes and soot, which in our case consists of molecules with more than 80 atoms) in axisymmetry. The following process conditions have been taken into account: temperatures of the anode and of the cathode, wall temperature, the geometry of the reactor chamber, inert gas type and density, initial species densities, current intensity, magnetic field density, gas velocity and species mass fraction. The following phenomena can be tackled by the model: evaporation of carbon from the anode, cathode surface deposition, species segregation, plasma jet transition and fullerene formation kinetics. The model gives mass, temperature, velocity and carbon mass species fields as well as fullerene growth rate and yield. The related set of strongly coupled partial differential equations is solved by using the local radial basis funtion collocation approach with multiquadrics shape functions, explicit time stepping, and five-noded influence domain. Several numerical examples are shown.