Application of an integrated CFD model to the metallic nanoparticle production in an Inductively Coupled Plasma reactor.

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A model has been developed to assist the design and operation of an inductively coupled plasma reactor process for the production of aluminum nanoparticles. The CFD (Computational Fluid Dynamics) open-source package OpenFOAM is used to solve the model's constitutive equations:

- Navier-Stoke, thermal energy, and mass diffusion equations
- Maxwell equations formulated as vector potential equations
- Lagrangian particle trajectory equations, including two-way coupling with the plasma flow
- Nanoparticle Population Balance Equation (PBE), formulated using the Method of Moments (MOM)

The model is used to optimize the operating conditions of the reactor: power, gas flow rates, aluminum precursor injection rates and gas quench configuration. A detailed study of the precursor injection is made, where it is shown that even for very low particle loading rations, i.e. 0.3 g/min of precursor particles, the local decrease of the temperature field in the plasma is still unexpectedly pronounced. While the relative mass loading is well below 1%, a decrease of more than 2000 K is still observed along the centerline of the plasma. The importance of the direct coupling plays a role, but most of the two-phase coupling is in this case due to the important changes in plasma properties and plasma radiation. An accurate prediction of the evaporation pattern of the precursor microparticles is shown to be critical in the operation of the reactor because of the strong effect of the type of quench used. A further study of the quench is made and enables us to identify the complex behaviour of the nanoparticle nucleation, growth and transport in the reactor. The critical importance of the flow, temperature, vapor concentration patterns on the nucleation and growth of the nanoparticles is clearly shown.

The model is used to predict particle size distribution from the first three moments of the particle size distribution, and furthermore predicts the agglomerated state of the particles, using two supplemental moments using fractal geometry.

Full results and references will be given in the full length paper.