THESIS PROPOSAL VSPARTICLE

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GOAL:

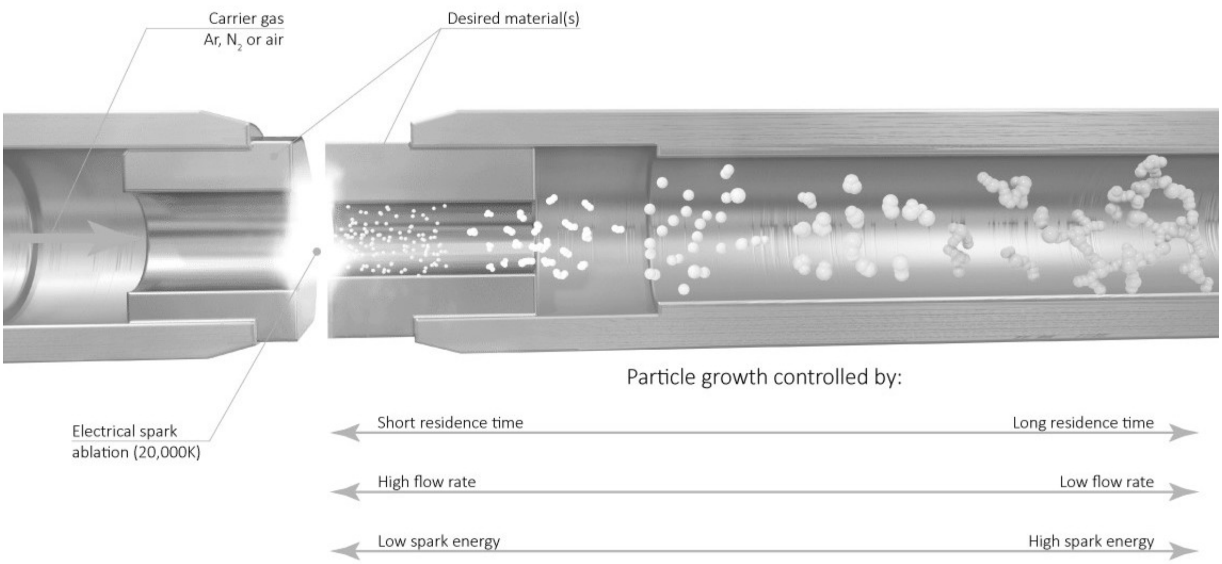
Develop an accurate and computationally efficient numerical model which describes the growth of nanoparticles from a gas produced by the VSP-G1.

SETTING

VSPARTICLE delivers user-friendly tools which can produce any inorganic nanoparticle. Nanoparticle production is key for the development of new materials for applications like sensors and microelectronics, but also for various fields of research. VSPARTICLE enables researchers to use particles smaller than 20 nm which are formed from a solid (semi)conductive electrode material.

VSP-G1

The technology used for nanoparticle production is a gas phase physical process called spark ablation. The inputs of the process are a conductive feedstock (e.g. Ag or Cu rod), electricity, and a carrier gas. A potential difference over the electrodes initiates ablation, resulting in a highly concentrated aerosol of pure (metal) gas suspended in a clean carrier gas as output.



Next, the aerosol is transferred through a tube allowing the particles to grow due to coagulation and agglomeration. Particle growth is dependent on the material, flow rate, tube length, and spark energy, but other parameters may also be of influence.

Generally, the particles are deposited onto a substrate. There are different forms of deposition. A stream of nanoparticles is guided along the surface and propelled to the substrate by inertia, diffusion or electrodeposition.

Computational modelling of nanoparticle production in the VSP-G1 is needed in order to get a better understanding of the influencing parameters in the process, and eventually to control the properties of the nanoparticles in the output.

RESEARCH GOALS:

1. Describe and model the whole nanoparticle production process, with emphasis on nanoparticle growth
2. Describe the influence of the parameters involved
3. Correlate the output of the models with experimental results
4. Recommend experimental improvements based on the parameters in the model

PLAN OF ACTION:

1. Develop the model in three steps:
    a. In order to mathematically describe the nanoparticle production process, it is essential to fully understand the VSP-G1 and the nanoparticle production process, with emphasis on nanoparticle growth due to processes like coagulation and agglomeration. Essential nanoparticle properties that we wish to control also need to be defined. A literature study will be done to understand theoretical processes like growth of spherical particles (coagulation), which will be the fundamentals of the mathematical model. Theory of non-spherical growth resulting in agglomerates will later be needed to expand the model and to improve in accuracy. Based on VSPARTICLE data the model is then adjusted to match assumptions and other processes specific for the VSP-G1.
    b. Next, an inventory is made of suitable modelling methods to convert the mathematical model to a numerical scheme. Methods to investigate include the moment of methods, the Monte Carlo method, the sectional method and possibly others. Criteria are: accuracy, computational cost, complexity and availability.
    c. Then, a method will be implemented to develop an accurate and efficient replication of the nanoparticle production of the VSP-G1 in Python. Possibly, different methods and techniques will be combined, or more than one model will be developed to test the performance of different methods. An essential output of the model will be the particle size distribution.

2. Perform a parameter sensitivity analyses and compare them with theoretical parameter influences. Possibly iterate to expand the model to improve accuracy and efficiency.

3. The output of the numerical model is to be correlated with experimental results. VSPARTICLE possesses a Differential Mobility Analyzer (DMA) that measures the particle size distribution. The DMA can be used to validate the model. Other, possibly better, validation methods may also be used, depending on availability, costs, and accuracy. Again, iteration takes place to expand the model to improve accuracy and efficiency.

4. Once the model suffices in accuracy and efficiency, recommendations based on parameters in the model can be made to better control the output of the VSP-G1.