SimDOME

User Story: An automated suite for the Gas-Phase nanoparticle synthesis simulation using an ICP reactor.

Aims

- Predict nanoparticles properties at reactor's output, given the reactor's configuration.

Methodology

- Integrating NanoDome models with a CFD software to enhance results accuracy.
- NanoDOME refactoring to improve usability, numerical stability and EMMO compliance.

Results

- Nanoparticles diameter, number density, fractal dimensions, PSD and internal structure using a standalone, a linked or a coupled approach.

Summary

Gas-Phase synthetized nanoparticles are gaining widespread popularity for the industrial use thanks to their enhanced properties with respect to a non-nanostructured material. NanoDome has been designed with the idea to offer a numerical suite which can be used as a Black-Box tool in the industrial context, offering three simulation methods of increasing complexity (MoM, PBM and CGMD). This user story describes NanoDOME's capability to evaluate the most relevant nanoparticle (NP) properties (diameter, number density, fractal dimension, internal structure etc.) using a standalone, a CFD-linked or a reactor network (CFD-coupled) method. An output example for CGMD is shown in *Figure 1*.

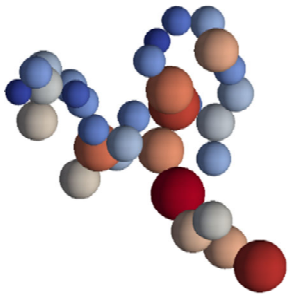

Figure 1: Example of NP internal structure with NanoDOME's CGMD [1]

Case Description

Following [1], an experimental ICP (Inductively Coupled Plasma) reactor has been chosen from literature (Tekna© PL-50), where an LTE plasma vaporizes a solid precursor (e.g., Ag, Al, Fe, etc.) which subsequently starts to form NPs while crossing a cooled chamber. The carrier gas is composed by a variable mixture of Argon, Hydrogen, Nitrogen and Oxygen. The final NPs properties are assessed at reactor's outlet with the preferred simulative approach.

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Developed methodology

For this case three simulation methods for NanoDOME are available: 1) Using it as standalone tool to simulate the case with a minimal set of inputs; 2) Linking it to a CFD software to account for different thermal evolution pathways, neglecting NPs effects on gaseous phase; 3) Coupling it to a custom 1D-CFD software to account for the precursor vapour phase transport phenomena inside the reactor.

In *Figure 2,* a schematic representation of the device used for methods 2) and 3) is shown. Regarding method 2), the operative conditions and plasma properties are computed with the *Elenbaas* code and passed to a CFD software (e.g., *OpenFOAM©*) to compute a set of streamlines (*Figure 2*) which are used by NanoDOME to evaluate the NPs evolution with one of the available models: Method of Moments (MoM), Population Balance Method (PBM) or Coarse-Grained Molecular Dynamics (CGMD). The same models are available for the method 1). In method 3), the computational domain is divided into a set of computational cells, each with a PBM NanoDOME instance exchanging data with the 1D-CFD solver at runtime. NanoDOME has also been refactored to be ontologically structured, in line with the latest EMMO release.

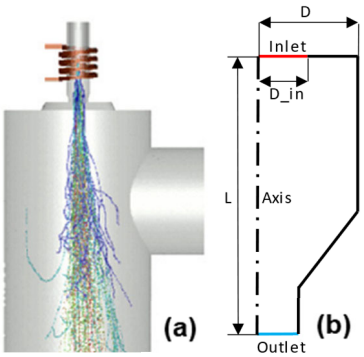

*Figure 2: ICP reactor schematization **(b)** and streamlines example **(a).***

Results

In Figure 3 the results, for all models, obtained for a reactor (D_in = 50 mm, D = 128 mm, L = 875 mm) operating at atmospheric pressure with a gas composition of Si 25% and Ar 75% and an ICP torch with an input power of roughly 25 kW are shown.

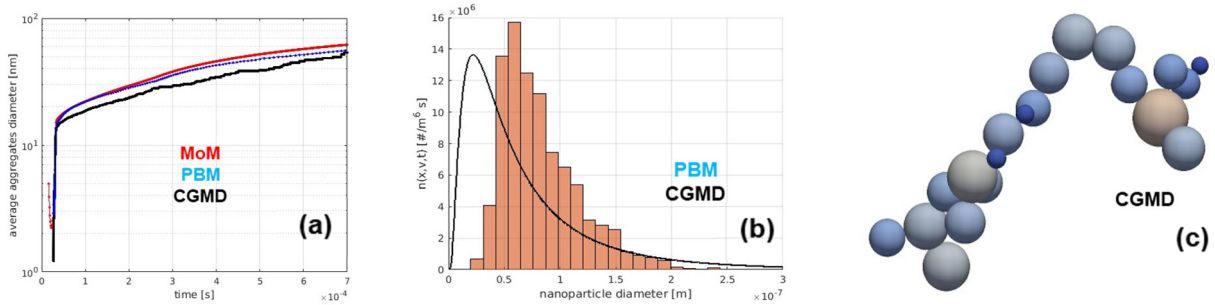

Figure 3: Results ordered for increasing NanoDOME's models accuracy:
***(a)** diameters time evolution, **(b)** PSD and **(c)** NP molecular structure at reactor's outlet.*

All models exhibit the same temporal evolution (Figure 3a), with a predicted mean diameter value at output of approximately 65 nm. PBM and CGMD models predict a PSD (Particle Size Distribution) with a log-normal shape centered at the above mentioned value (Figure 3b). The CGMD also computes a final mean fractal dimension value of about 1.45. In Figure 3c the molecular structure graphical representation for a specific nanoparticle is shown, with fractal dimension comparable to the computed mean value. The results are in good matching with the experimental results available in [1].

References

[1] F. Strappaveccia and F. Galleni and E. Ghedini, "H2020 NanoDome Project: A Unified Approach for Gas-Phase Nanoparticles Synthesis Modelling", *Journal of Physics: Conference Series,* vol. 1243, p. 012018, May 2016. DOI: 10.1088/1742-6596/1243/1/012018

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