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Modelling of "Hetero-Aggregation" of Different Particle Types

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Nanoparticles are known for their unique physical and chemical properties, which often differ significantly from their bulk material counterparts. These special characteristics have made nanoparticles essential in various industries, ranging from energy storage in batteries to advanced materials like ceramics, emulsions, and electrolytes. Beyond their individual properties, recent research has revealed that nanoparticles can exhibit even more complex behaviors when they form hetero-aggregates—composite particles composed of two or more distinct phases.

Hetero-aggregates can be formed during mixing of aerosol streams. This method is advantageous due to its compatibility with gas-phase synthesis techniques, making it a promising approach in industrial-scale production. However, the formation dynamics of these hetero-aggregates – encompassing nucleation, condensation, coagulation, and the mixing of cooled aerosol products – are strongly influenced by the surrounding gas environment. Despite their importance, these processes are not yet fully understood.

Tracking the composition of the hetero-aggregate introduces an additional dimension into the population balance equation (PBE) making its solution via classical sectional model extremely expensive. Therefore, we propose a new, simplified model based on the monodisperse framework, enabling it to describe the growth of hetero-aggregates formed from the interaction of two or more particle streams. This hetero-monodisperse model is specifically designed for integration with computational fluid dynamics (CFD) methods, particularly the Eulerian-Lagrangian decomposition (ELD) approach, which is optimized for high Schmidt-number flows.

The hetero-monodisperse model accounts for various mechanisms critical to hetero-aggregate formation, including binary and unary nucleation, inter- and intra-population coagulation, and condensation. Its performance was validated against an established two-dimensional sectional model previously proposed by Shigeta and Watanabe for plasma reactor applications. Comparative testing in scenarios involving Mo–Si and Ti–Si systems demonstrated that the new model could accurately capture the evolution of critical parameters such as particle number concentration, volume, and composition.

One of the most significant advantages of the hetero-monodisperse model is its computational efficiency. In benchmark simulations, it achieved a speed-up of over 6,000 times compared to the nodal model while maintaining comparable accuracy. This remarkable efficiency makes it a highly practical tool for simulating hetero-aggregate dynamics, especially in complex three-dimensional environments where traditional models would be computationally prohibitive.

Furthermore, the hetero-monodisperse model is not limited to two-material systems. An extended version of the model, outlined in matrix form, can accommodate systems with more than two materials, making it a versatile tool for a wide range of industrial and research applications. Its compatibility with both commercial and open-source CFD platforms further enhances its utility, allowing researchers and engineers to simulate and analyze hetero-aggregate formation.