Quantification of the mixing zone and intensification of the mixing process of two nanoparticle producing flames for the design of hetero-contacts

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In Short

- Synthesis of Nanoparticles
- Flame Spray Pyrolysis
- Mixing Processes
- Hetero-Aggregates
- Hybrid RANS/LES

The shift to clean energy poses a lot of challenges for modern society, tailormade particles on a nanoscale can help here with tailormade characteristics. Nanoparticles hold great promise for transforming industrial applications, such as batteries, catalysts, sensors, and super magnetic materials. Especially the hetero-aggregates with their hetero contacts hold here potential as they allow for specific charge distribution. This is the reason why the quality of these hetero-aggregates is also dependent on the number of hetero contacts within the aggregate. The investigation of these hetero-aggregates is also part of the DFG- funded priority programm SPP 2289, where the formation and implementation of hetero- aggregates is investigated. The double flame spray pyrolysis (DFSP) combines two nanoparticle producing flames. The separate control of the particle formation and growth in each flame via the process parameters before reaching the mixing zone makes DFSP an attractive route for the synthesis of functional catalysts from the gas phase. Here the transport of heat, charge carriers or surface species across the interface determines the functionality of the mixed system. By adjusting the DFSP process parameters such as intersection distances and angles, it is possible to meet the specific requirements of various multi-component catalysts for Fischer-Tropsch synthesis [1], catalytic CO oxidation[2], dry reforming [3] and recently lithium ion batteries [4]. The objective of this project is to comprehend the relationship between the mixing zone and the mixture state of aggregates, including the necessary hetero-contacts. The mixing of the two flames remains a mystery, and as shown in Figure 1, different configurations lead to vastly different products from the double flame.

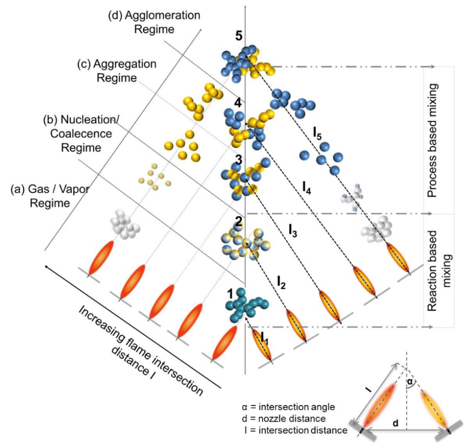

***Figure 1:** Influence of the Intersection distance on the resulting Mixture State [5].*

To enhance the understanding of the mixing processes of the double flame, a numerical investigation of the entire setup will be conducted. The simulations are being conducted using OpenFOAM v2112. To gain a better understanding of the mixing, a Large Eddy Simulation (LES) would be ideal. However, due to their high computational cost and the fact that the simple flame spray has been extensively studied, a hybrid RANS/LES approach has been selected. As shown in Figure 2, the domain is divided into two theoretical sections: the Reynolds Navier Stokes (RANS) part from the nozzles down to the mixing zone, and the mixing zone itself. This approach offers the best of both worlds by providing the desired resolution for understanding the mixing processes in the mixing zone, while still being computationally efficient in the areas where it is affordable.

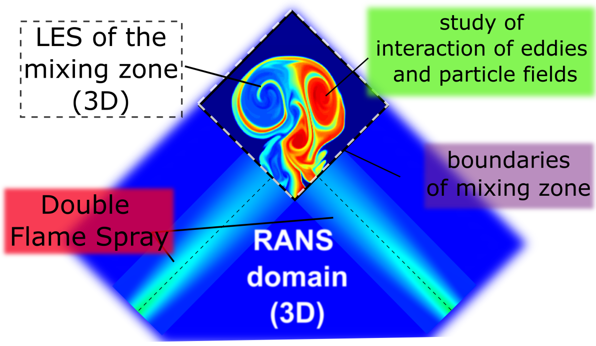

***Figure 2:** Numerical domains of the DFSP reactor.*

The aim of this numerical investigation is to generate design rules for tailormade nanoparticles and an increase in the number of hetero contacts based on the resulting quantification and understanding of the mixing zone. To achieve this, different DFSP setups with varying intersection angles, distances to the intersection, distances of the nozzles, and different nozzle pressures are examined.

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More Information

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DFG Subject Area

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