Motivation
• Identification of the particle formation mechanism on molecular scale including particle nucleation, particle growth and droplet exchange
• Investigation of the complex redistribution behavior of reactant ions
• Analysis of the influence of hydrodynamics on the particle formation

Modeling & Simulation Results
Assumptions:
1. The reactor is ideally macro-mixed
2. The water content of particle-free droplets and droplets with particles below the barrier size is monodisperse (equal water volume)
3. At maximum there exists only one particle per droplet
4. No agglomeration or breakage of particles

Model Reduction [2]:
\[ \frac{dP_{eq}(N_A, N_B, t)}{dt} = \frac{1}{N_A} \left( P_{BA_{feed}}(N_A, N_B,t) + P_{BA_{growth}}(N_A, N_B,t) - P_{BA_{nuc}}(N_A, N_B,t) \right) \]

2d + 1d - Model:
\[ \frac{dF_{BA_{growth}}(N_A, N_B,t)}{dt} = f_{BA_{growth}}(N_A, N_B,t) \]

Balance for particle-free droplets:
\[ \frac{dF_{BA_{feed}}(N_A, N_B,t)}{dt} = f_{BA_{feed}}(N_A, N_B,t) \]

Balance for the droplet number distribution with particles:
\[ \frac{dF_{BA_{nuc}}(N_A, N_B,t)}{dt} = f_{BA_{nuc}}(N_A, N_B,t) \]

Droplet exchange term:
\[ p_{BA_{nuc}}(N_A, N_B, t) \]
\[ p_{BA_{growth}}(N_A, N_B, t) \]
\[ p_{BA_{feed}}(N_A, N_B, t) \]

Experimental Results [1]

Collaborations
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Publications