Direct Numerical Simulation of Fluid Flow and Particle Formation Dynamics

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Excellent collaboration

Profs. M. Avila U Bremen, M. Manhardt, TUM

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AiF

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MehrDimPart SPP 2045

EAM ENGINEERING OF ADVANCED MATERIALS

DESIGN OF PARTICULATE PRODUCTS

Supporting companies

BAYER Bayer

CLARIANT

LANXESS

Product design of nanoparticles

Product and **property design**:

Property	= F (dispersity, composition)	**property function**
Dispersity	= G (process variables)	**process function**

Colloborative Research Center (CRC) 1411: Design of Particulate Products
with exemplary focus on design of optical properties of nanoparticles (NPs)

Lycurgus cup

Quantum dot display

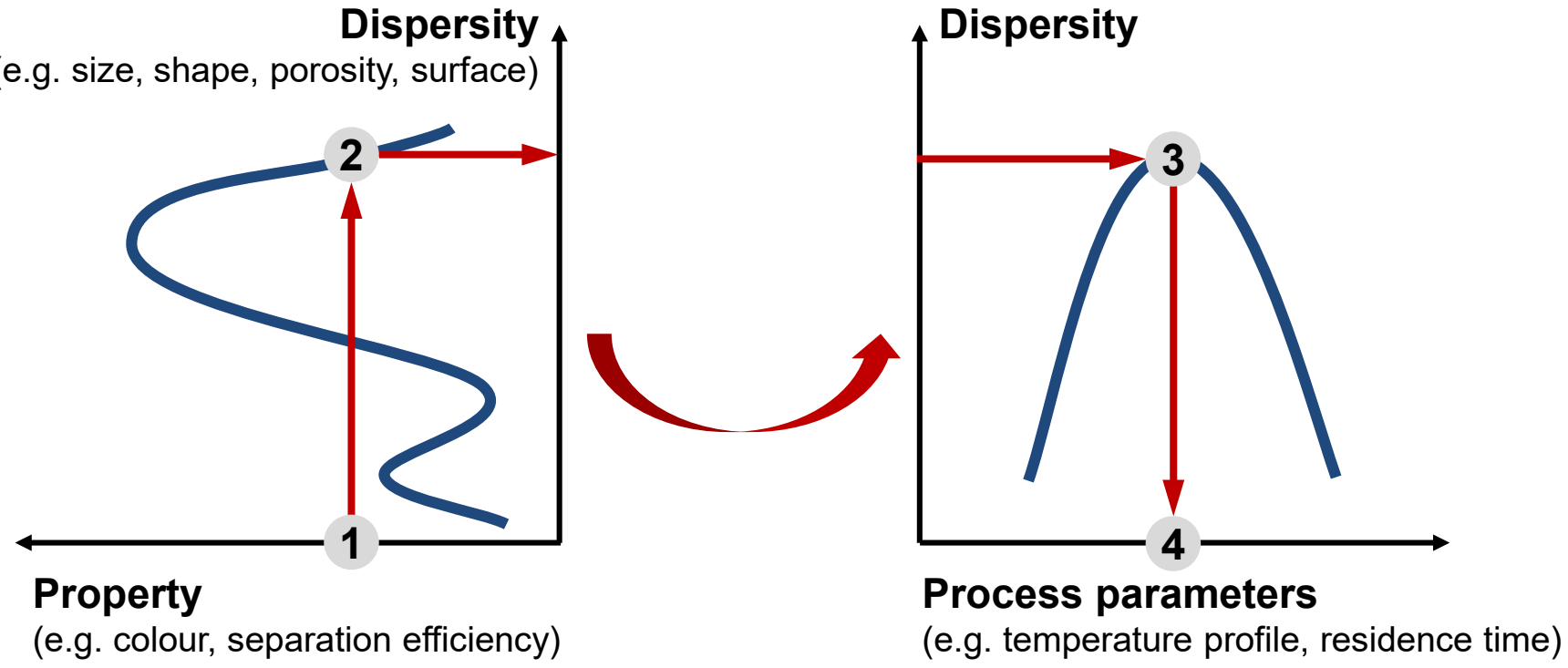
Structural colours

Challenges for the design of nanoparticulate products:

- Large gap between synthetic protocols and technical application
- Missing process technologies for NPs, their predictive design and scale-up

Predictive design:
From properties to processes ….

…. via rigorous mathematical optimisation based on predictive models



Principles of particle synthesis

Available techniques:

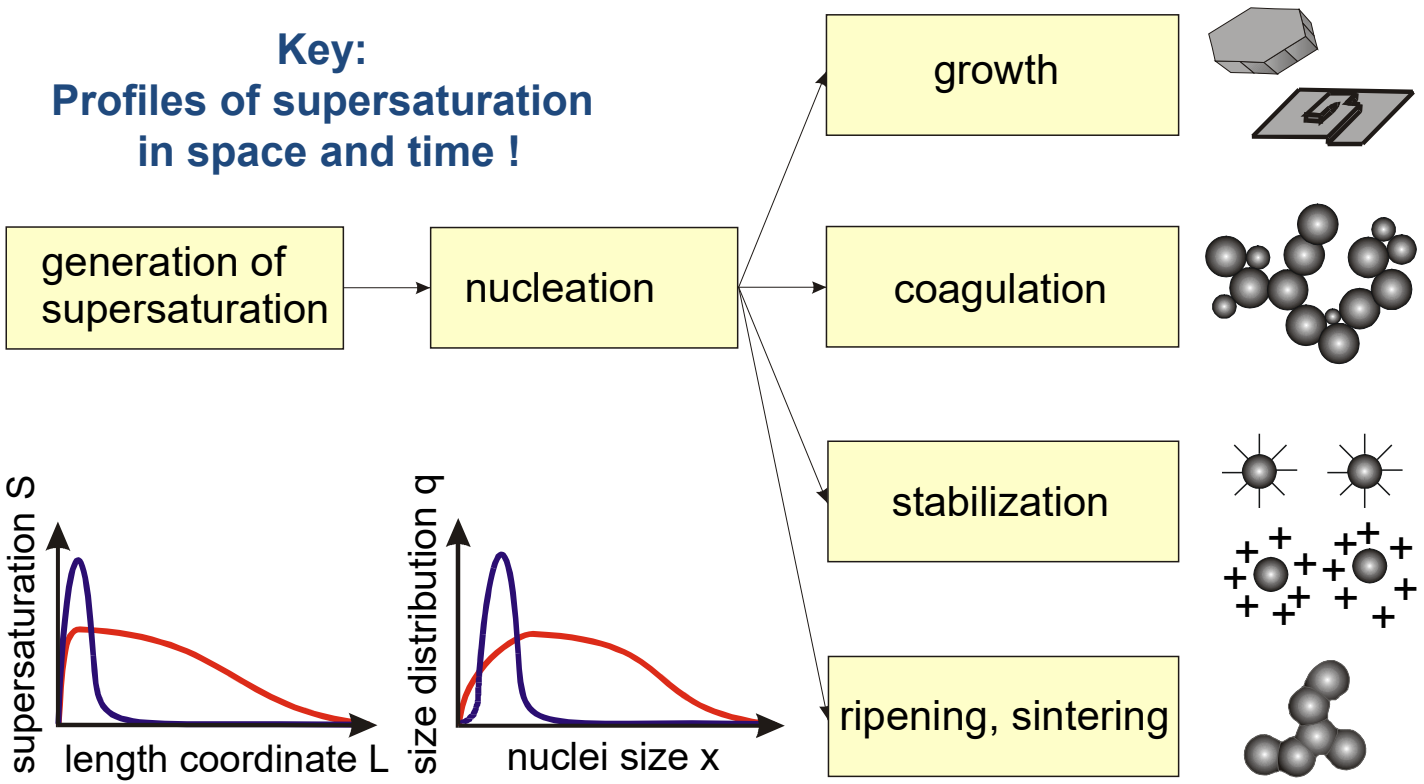
- Hot wall, spray flame, plasma, sparc discharge (gas phase)
- Hot injection, solvothermal, continuous precipitation, crystallization (liquid phase)

mass, momentum and heat transfer, chemical reactions

phase transition

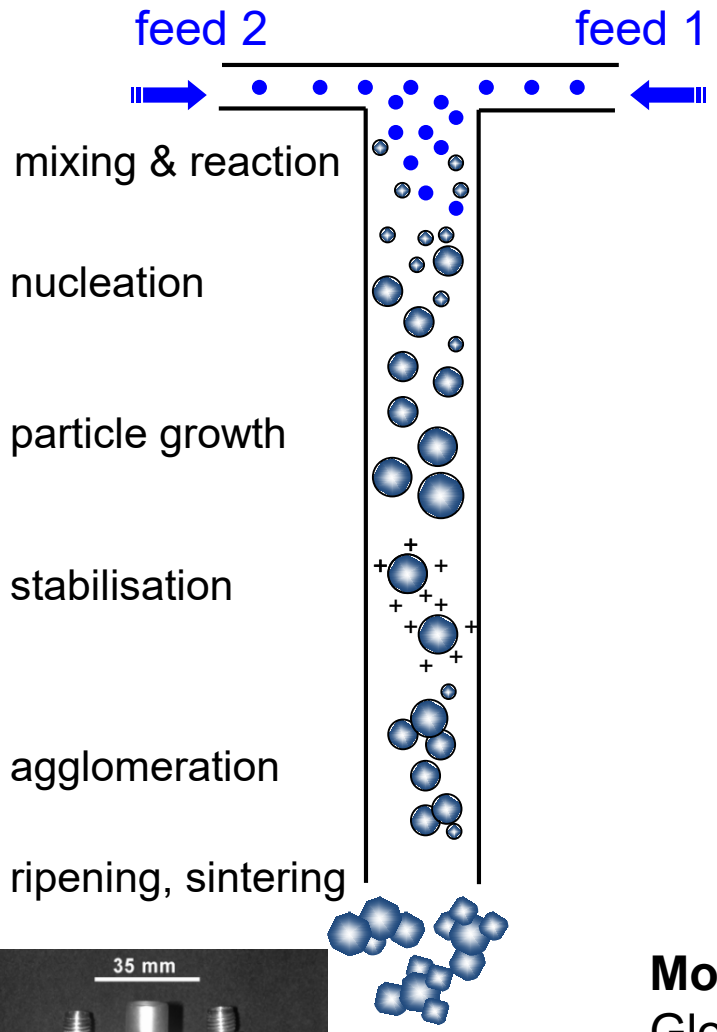
transfer processes interfacial process engineering

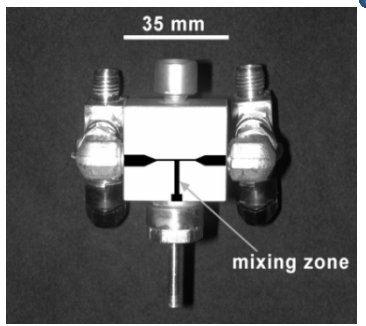
Key:
Profiles of supersaturation in space and time !



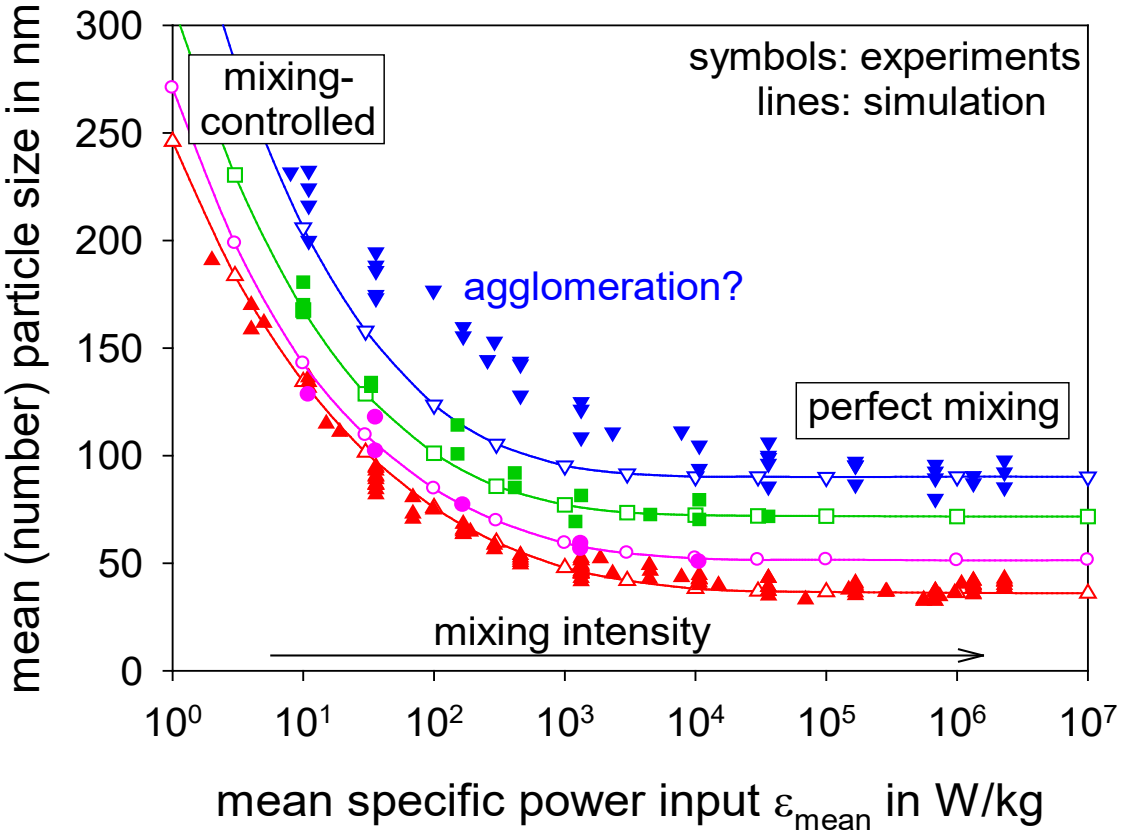
Peukert et al, Adv. Chem. Eng. 2015

Continuous particle synthesis in liquids





Precipitation of $BaSO_4$



Modelling:

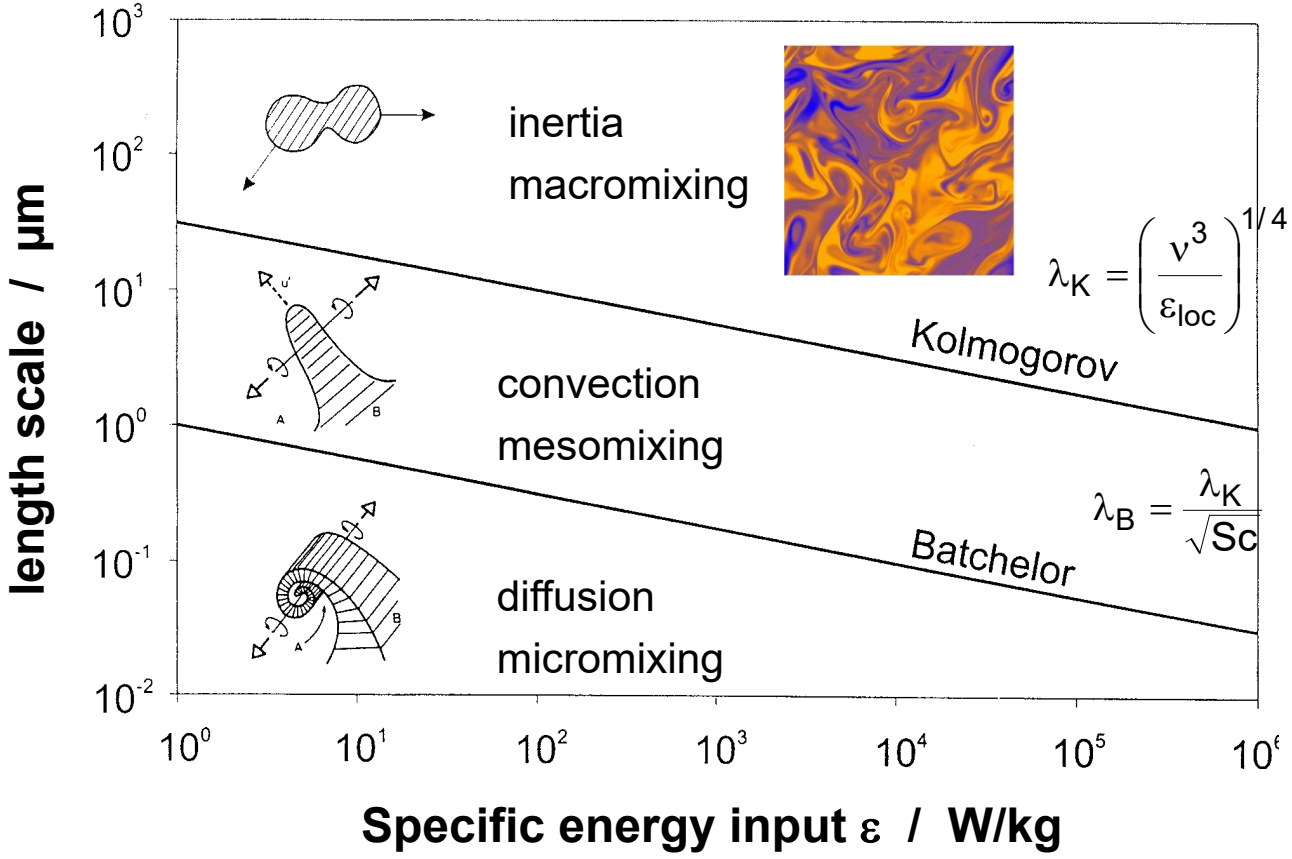
Global: mixing = f(Δp) + PBM

DNS + PBM along Lagragian tracks → x_{50}, full PSD

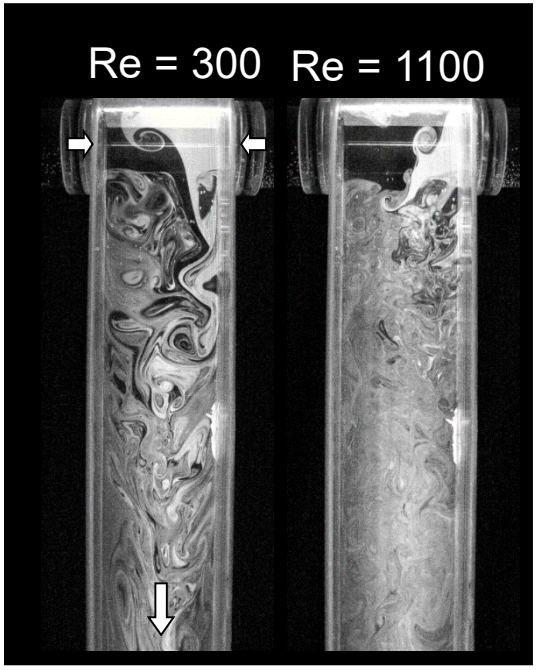
Schwarzer et al, AIChE Journal 2004, CES 2005, Gradl et al. CES 2009

Homogenizing for chemical reactions

Mixing influences fast chemical reactions & conversion of precursors



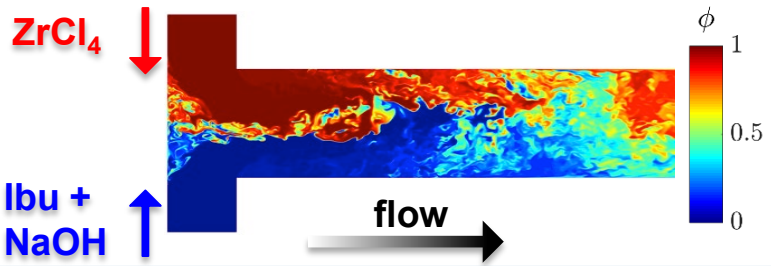
Mixing in micromixer
LIF measurements



- DNS allows resolution of fluid flow down to Kolmogorov scale
- In T-mixer full resolution down to a few µm
- Diffusion-controlled micromixing at small scales where the reactions occur
- Small mixing times (O ~ µs….ms) for NP production requires high energy input

Simulation framework

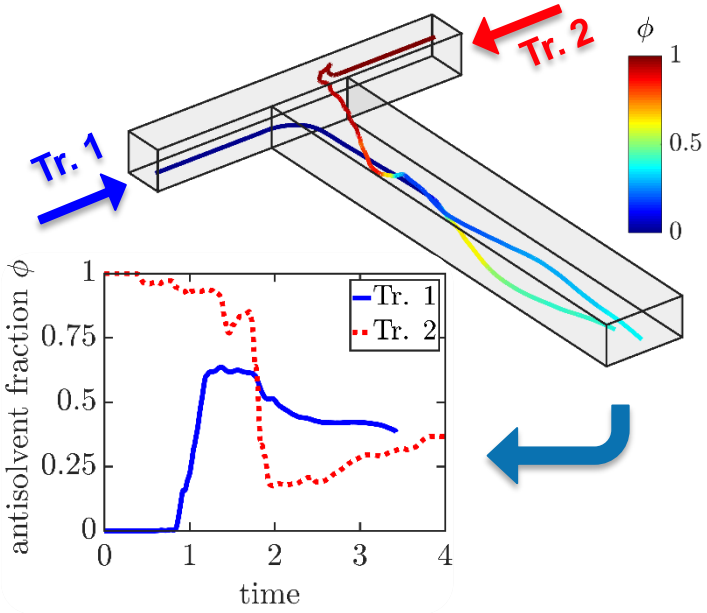
Simulation of flow field (in Eulerian space)



$\phi(\vec{x}, t)$

$u(\vec{x}, t)$

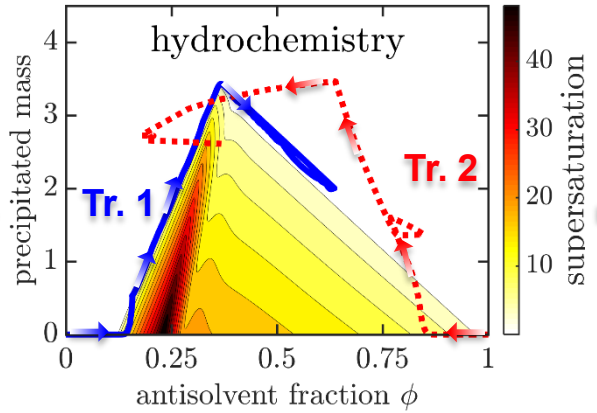
Decoupled mixing history (in Lagrangian space)



Tr. 1

Tr. 2

Modeling of precipitation (mixing history and hydrochemistry)



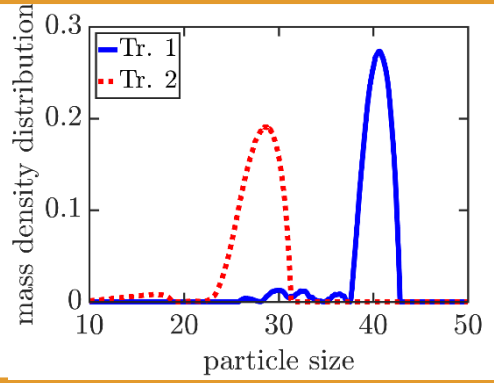
precipitated mass

supersaturation

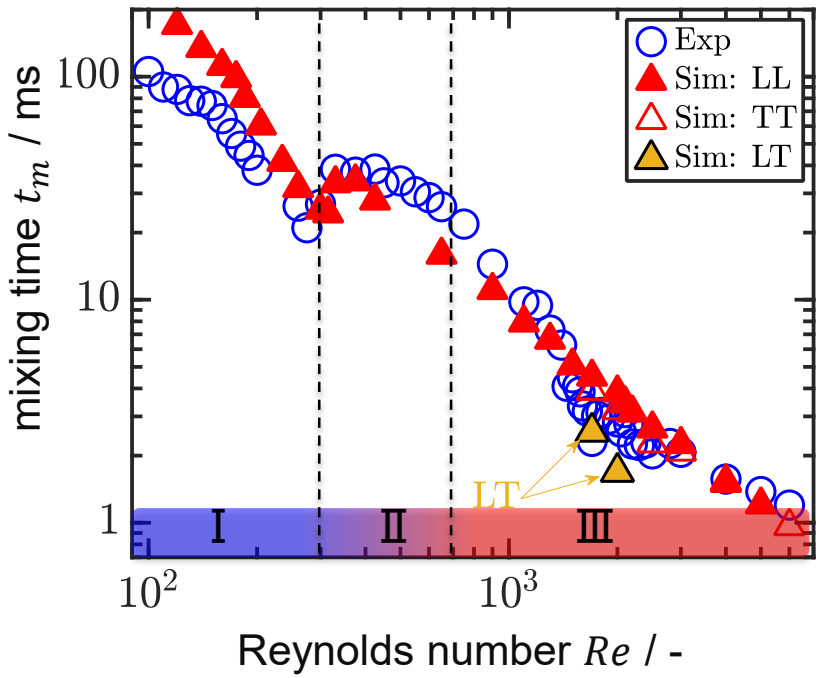
population balance equation

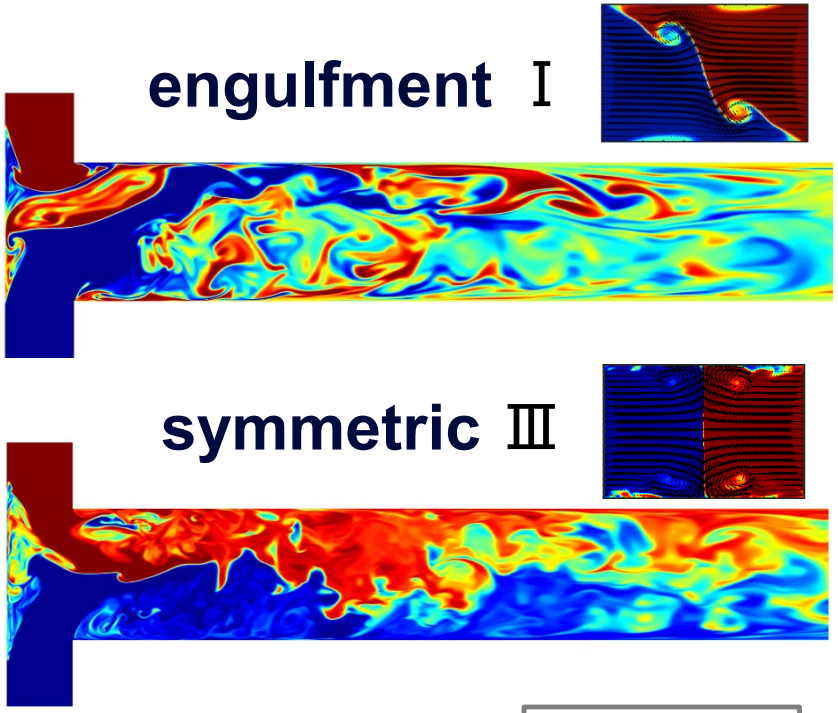
Result

Particle size distribution



Mixing in T-mixer: Flow structures





I low Re
II transition
III turbulent

Mixing determined by large flow structures

I. Different flow field instabilities (low Re)

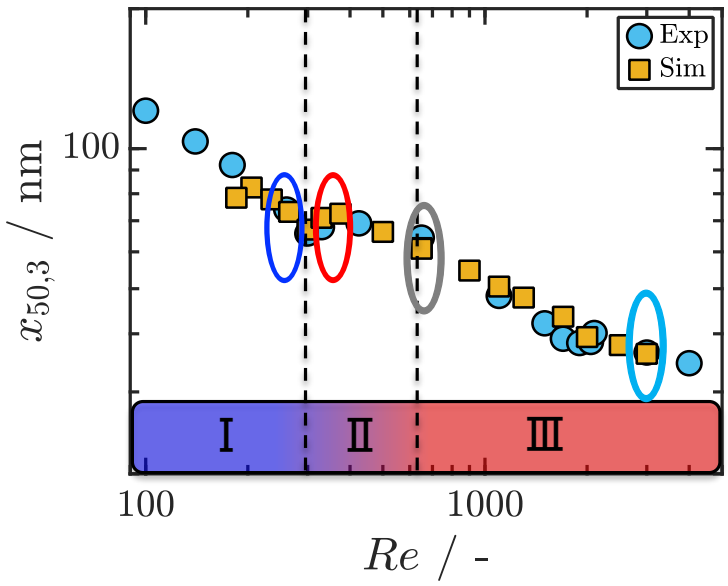
II. Various inflow conditions (**L**aminar-**L**aminar, **T**urbulent-**T**urbulent, **L**aminar-**T**urbulent)

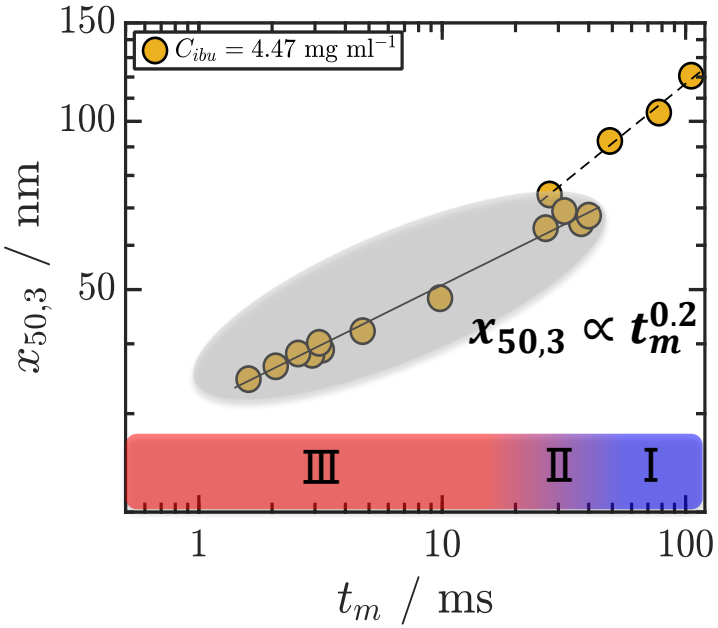
Mixing scales with mean energy input E_V

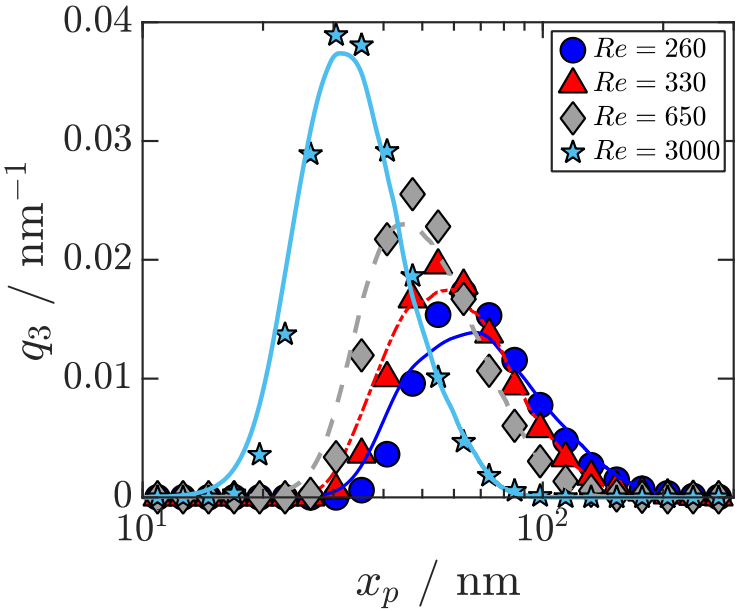
$$t_m \propto E_V^{-0.48}$$

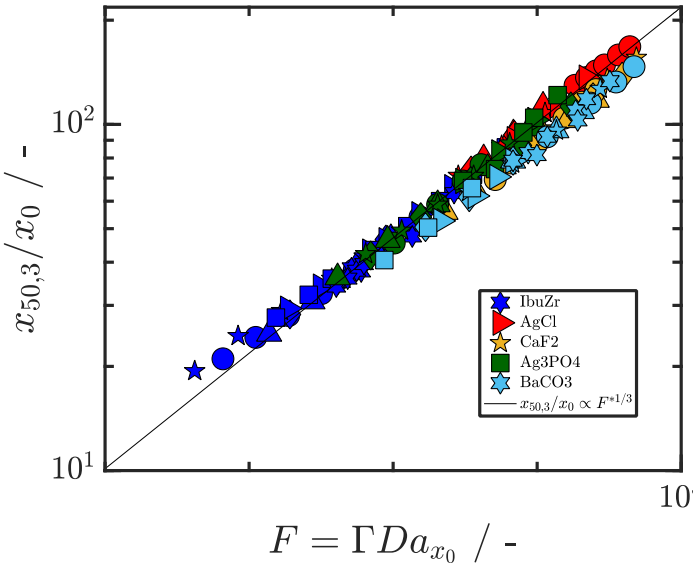
Schikarski, Trzenschiok, WP, Avila, ***RCE,*** *2019*

Case study: Ibuprofen stabilized by Zr-complexes



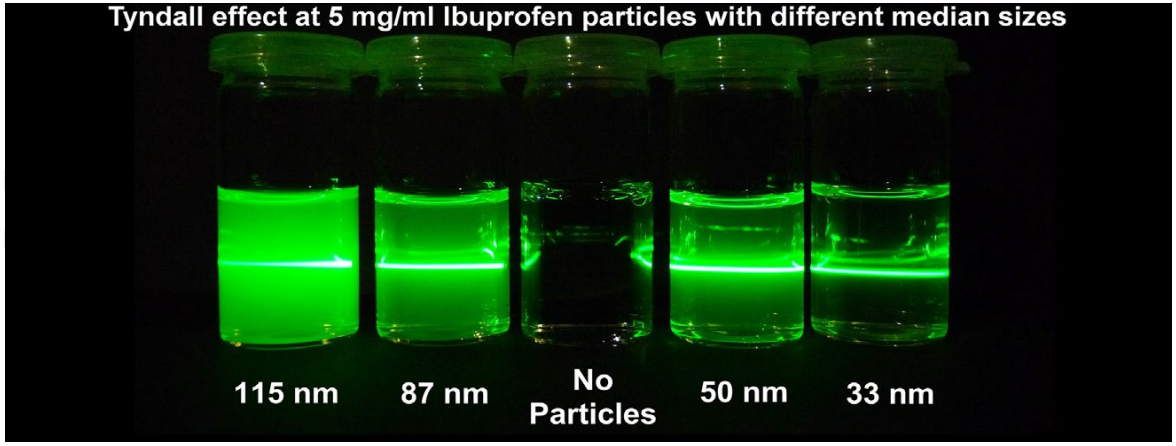






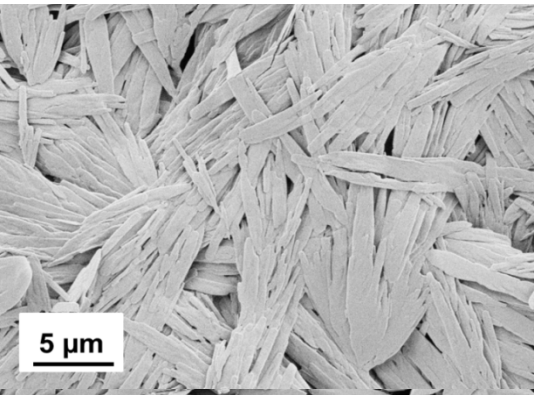
Schikarski, Avila, WP, Chem.Eng.J. 2022

Stabilization by complex formation

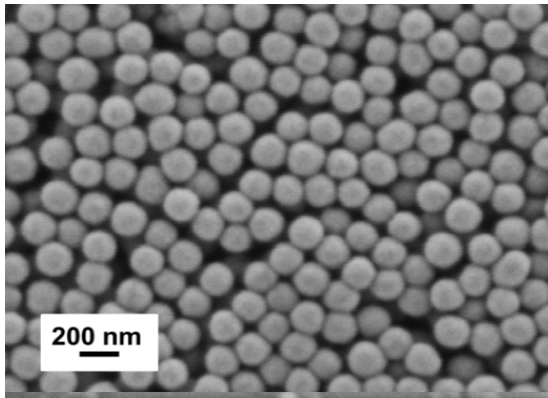


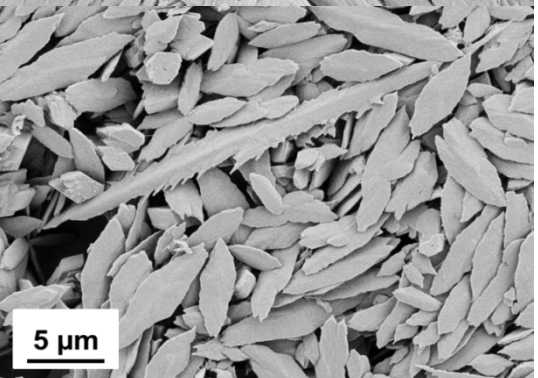
Traditional: Polymeric stabilizers

New: Fast charge stabilization

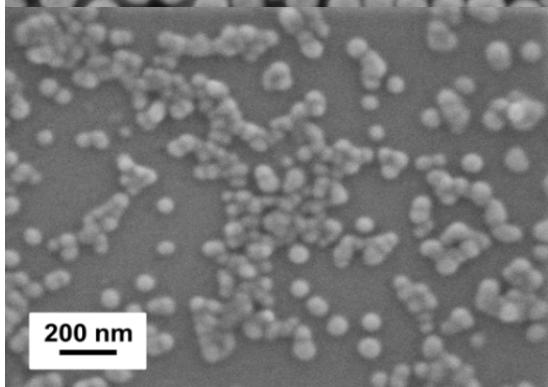


Naproxen



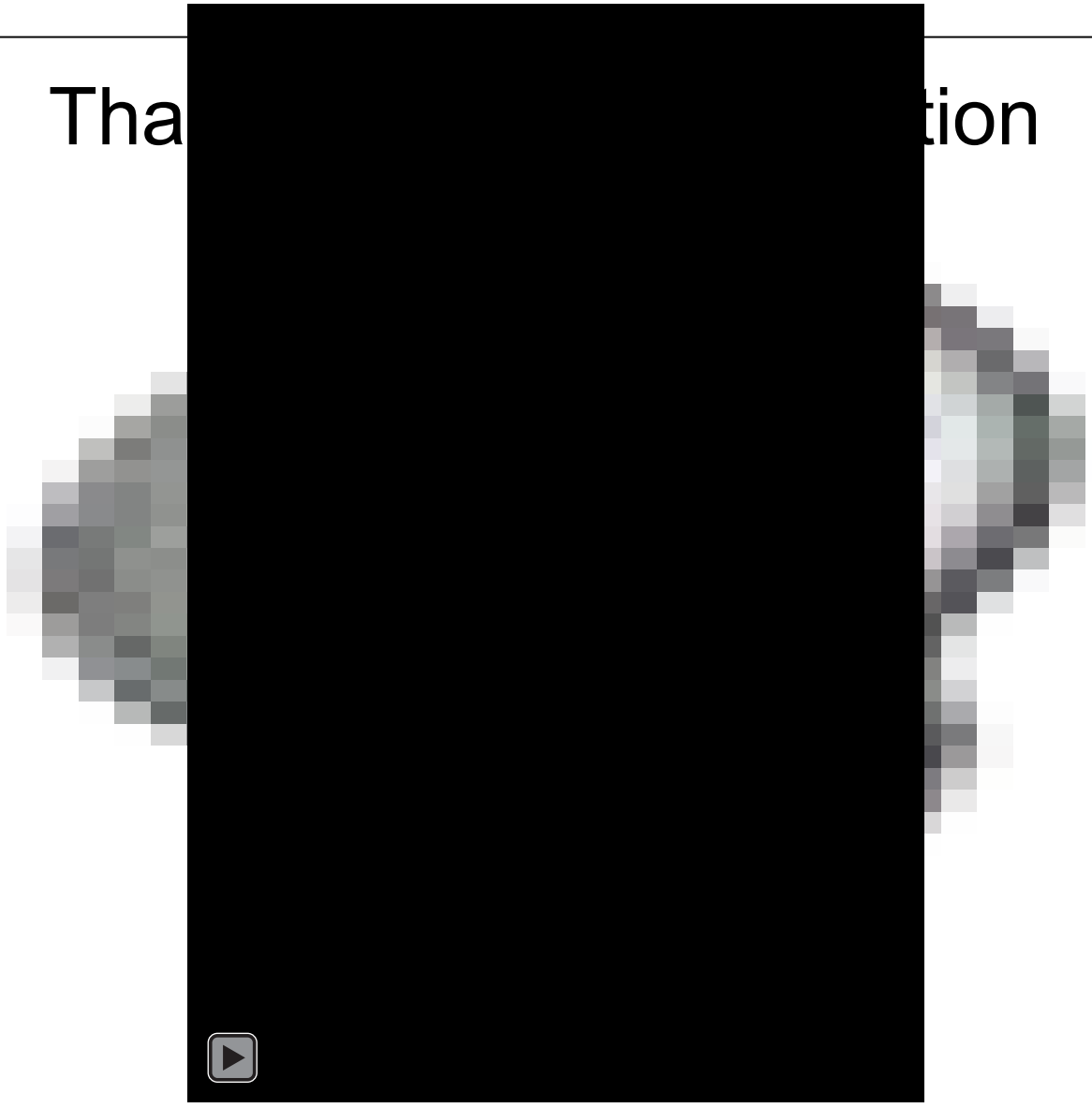


Mefenamic Acid



Trzenschiok, Schikarski, Avila, WP, Chem.Eng.J. 2018

Tha tion

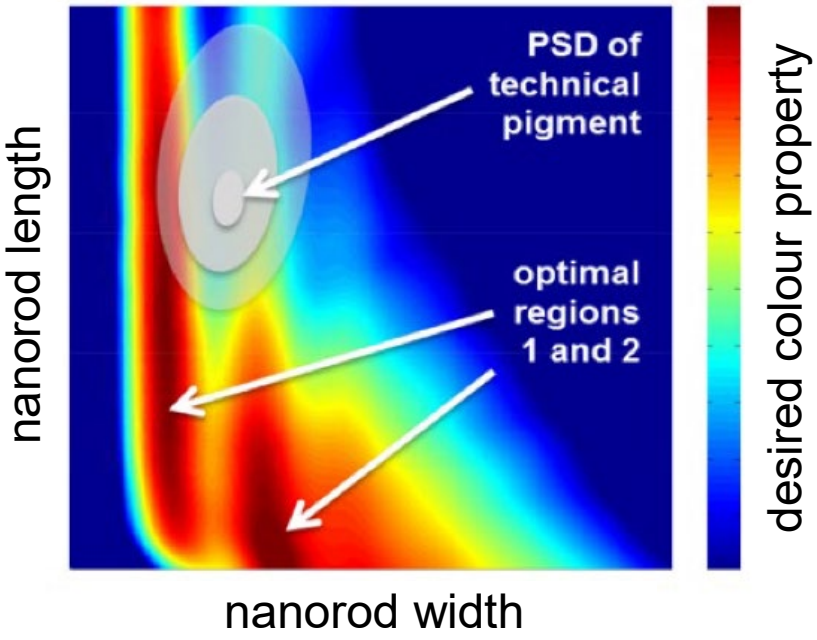


Optimal Property-structure-process functions

From properties to processes ….

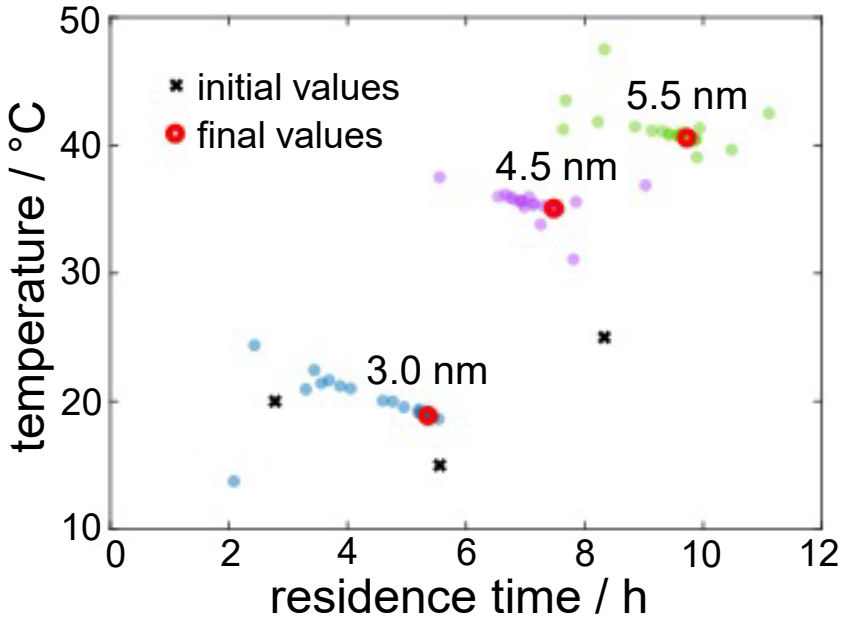
…. via rigorous mathematical optimisation based on predictive models

Optimal colour for FeOOH rod-like particles



Cooperation Klupp Taylor, Peukert, Pflug, Stingl with Lanxess. Two patents pending.

Optimal process parameters for ZnO quantum dots



Segets, Pflug, Peukert et al., Chem. Eng. J. 2015