2026 AIChE ANNUAL MEETING

NOVEMBER 8 - 12, 2026
MINNEAPOLIS, MN



CHEMICAL ENGINEERING **REIMAGINED**

Institute of Hydrology of the CAS

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Bridging scales in flocculation kinetics: From interparticle forces to turbulent flow

O. Gebouský[1,2], J. Haidl[1], V. Bílek[1,2], M. Pivokonský[1]

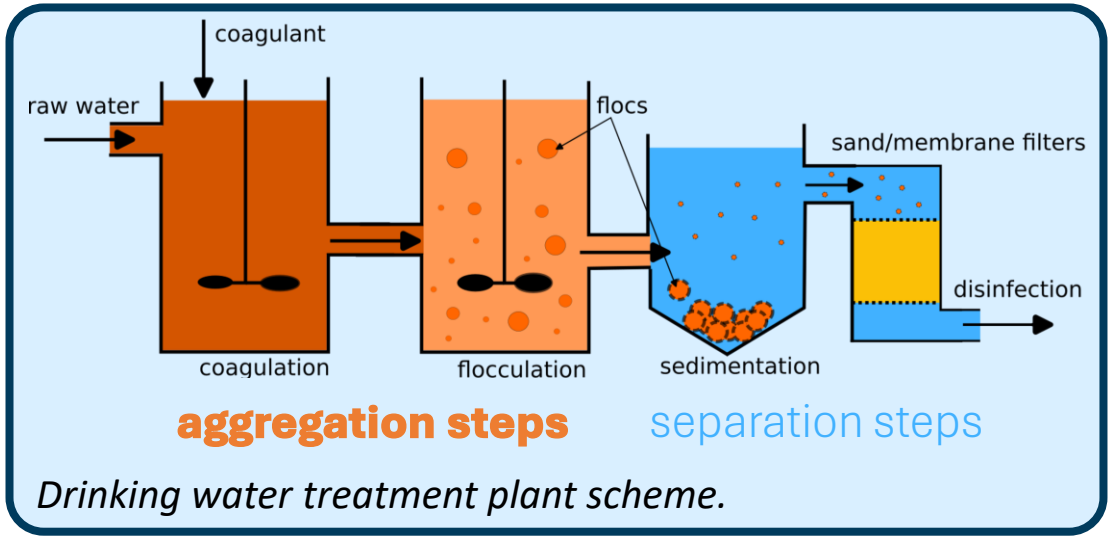
[1]Institute of Hydrology of the CAS, Pod Paťankou 30, 160 00 Prague 6, Czech Republic

[2]University of Chemistry and Technology, Technická 5, 166 28 Prague 6, Czech Republic



Motivation

- **Increasing water-quality challenges:**
  Emerging pollutants & stricter regulatory limits.
- **Need for aggregation steps understanding:**
  Aggregate properties govern subsequent separation and treatment efficiency.
- **Aggregate formation couples chemistry and mixing:**
  CFD provides the flow conditions for PBM-based prediction of aggregates size and morphology.



Drinking water treatment plant scheme.

Overall Objective

coupled **CFD–PBM model** for predictive simulation and coagulation/flocculation process design and optimization

Current Objetive

development, implementation and experimental validation of **Population Balance Model (PBM)**

Motivation

Taylor-Couette reactor experiments

- water + coagulant + impurities → flocs
- main findings:
  - unknown size d_0 and count N_0 of primary particles

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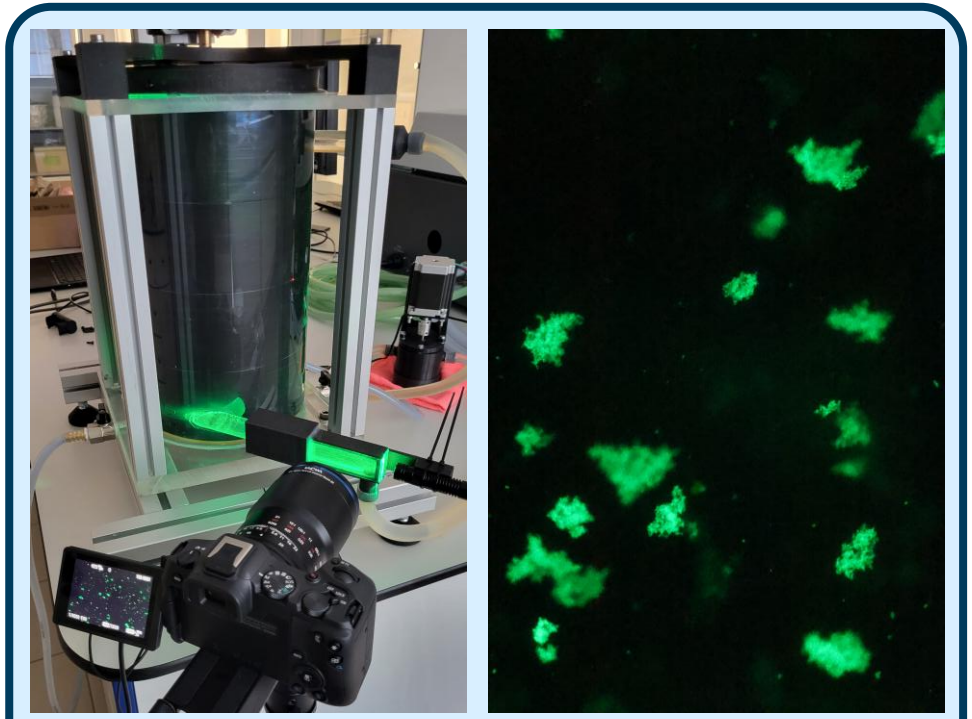
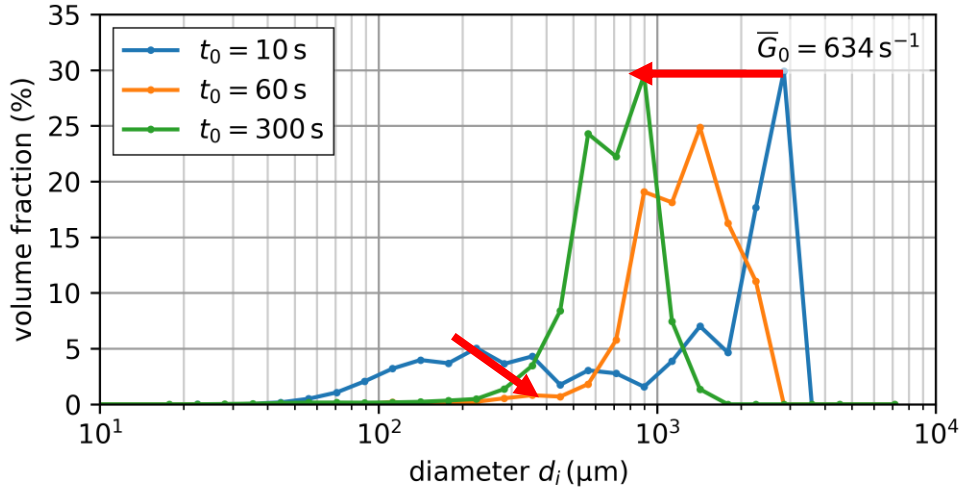
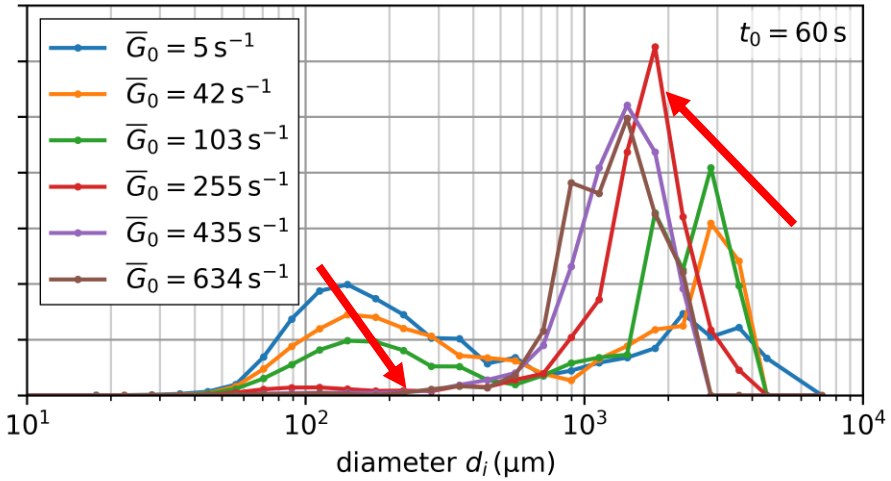
two more fitted parameters of PBM

  - dependence on duration t_0 and intensity $\overline{G}_0$ of rapid mixing



Taylor-Couette reactor, flocs in measuring cell.

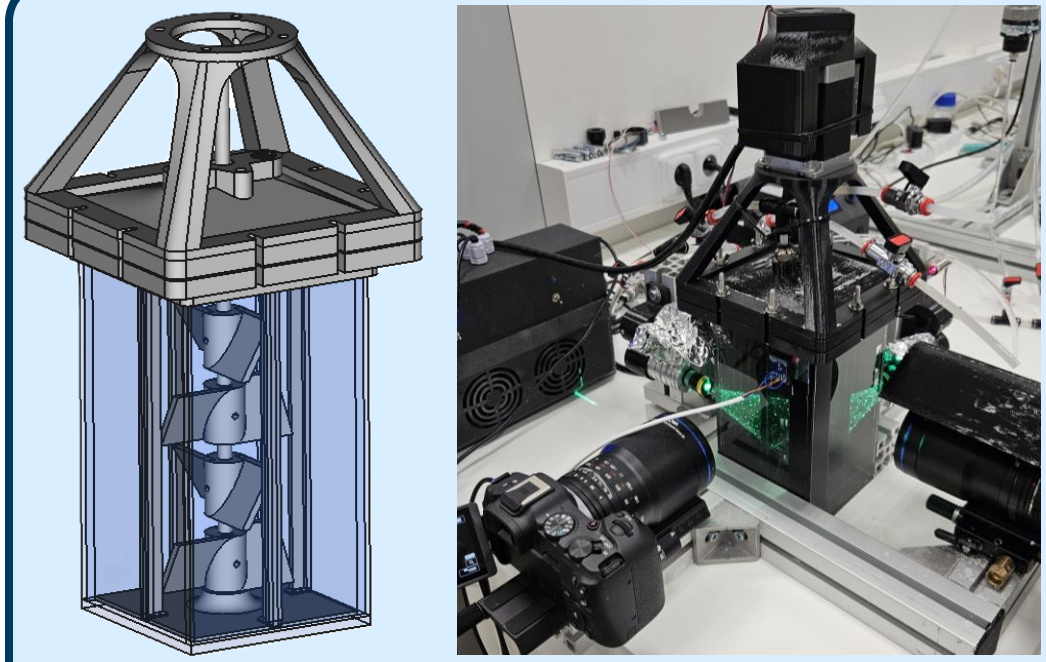




Motivation

Population Balance Modeling reactor

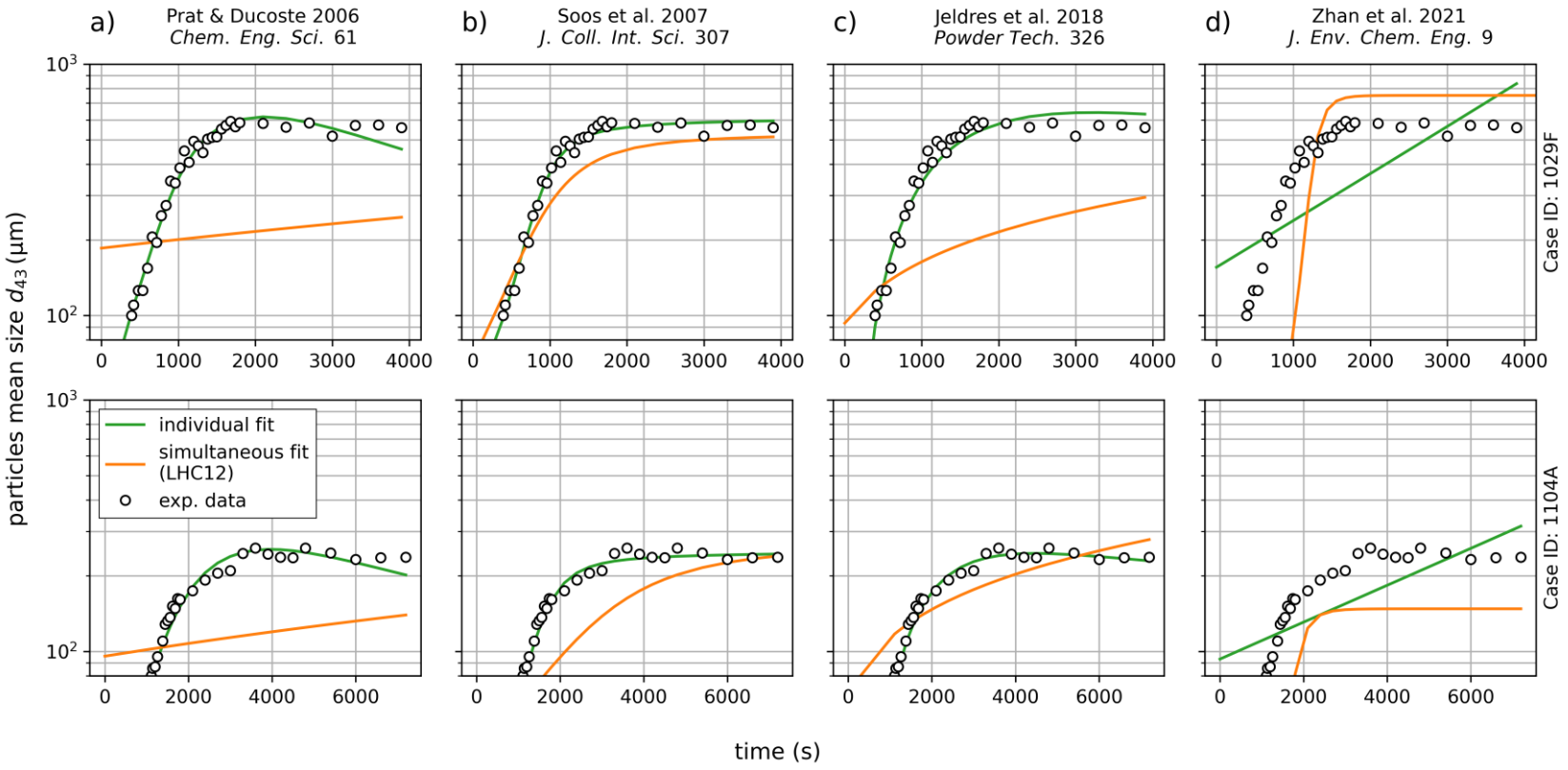
- PBM reactor ($V = 2.3$ L)
- physical, well-defined system
- polystyrene latex ($d_0 = \{0.1, 1.1\}$ μm) + aqueous NaCl solution
- five concentrations of solids:
  $c_s = \{10, 20, 30, 40, 80\}$ mg/L
- six mixing intensities:
  mean shear rates $\bar{G} = \{9, 13, 21, 31, 52, 77\}$ s^{-1}
- 60 experiments



Scheme and photo of PBMR.

Motivation

PBM in literature and identified drawbacks



Too specific experimental conditions and form of PBM model.

Insufficient set of exp. data for validation.

Model is not universal and transferable to our experimental data.

Population Balance Modeling

Model

$$\frac{\mathrm{d}N_k}{\mathrm{d}t} = \underbrace{\sum_{i=0}^{k}\sum_{j=0}^{i} A_{i,j}\,\kappa_{k,i,j}N_iN_j}_{\text{aggregation of smaller particles}} + \underbrace{\sum_{i=k}^{M} B_i\,N_i}_{\text{breakage of bigger particles}} - \underbrace{\sum_{i=0}^{M} A_{k,i}\,N_kN_i}_{\text{aggregation to bigger particles}} - \underbrace{A_{k,k}N_k^2}_{\text{aggregation to bigger particles}} - \underbrace{B_kN_k}_{\text{breakage to smaller particles}}$$

growth **loss**

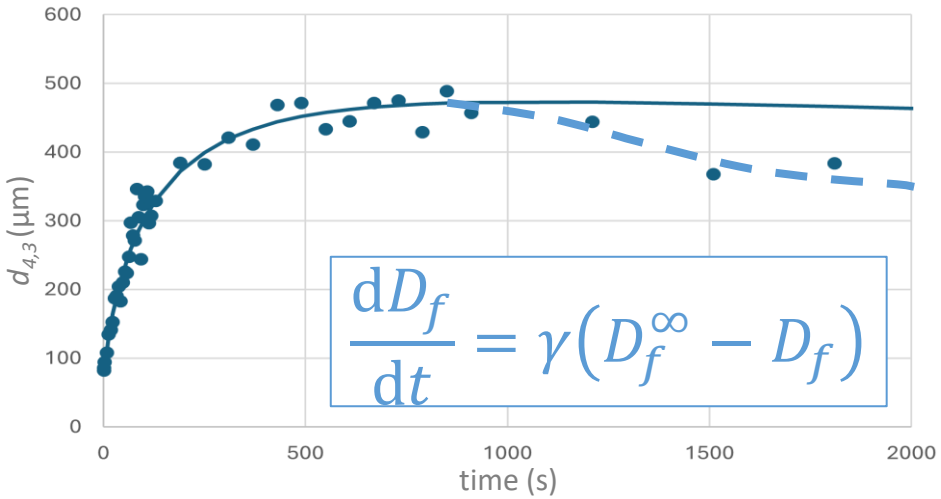
- aggregation kernel $A_{i,j}$
- breakage kernel B_i
- mass conservation factor $\kappa_{k,i,j}$

- mass and diameter of primary particle – m_0, d_0
- mass of subsequent classes – geometric sequence with $\omega = 2$

$$m_k = m_0\omega^k, \qquad k = 0\,..\,M$$

- fractal aggregates with characteristic diameter and mass fraction

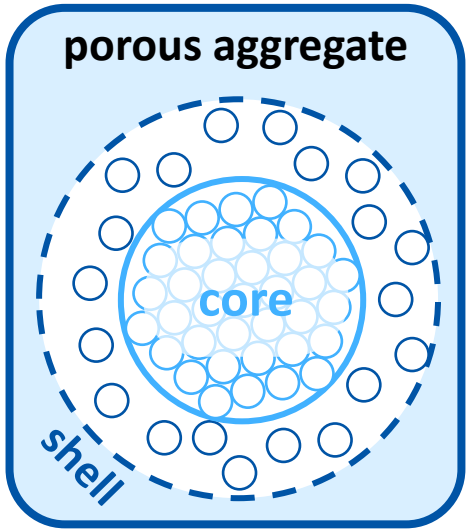
$$d_k = d_0\omega^{1/D_f}, \qquad \phi_k = (d_k/d_0)^{D_f-3}$$



Population Balance Modeling

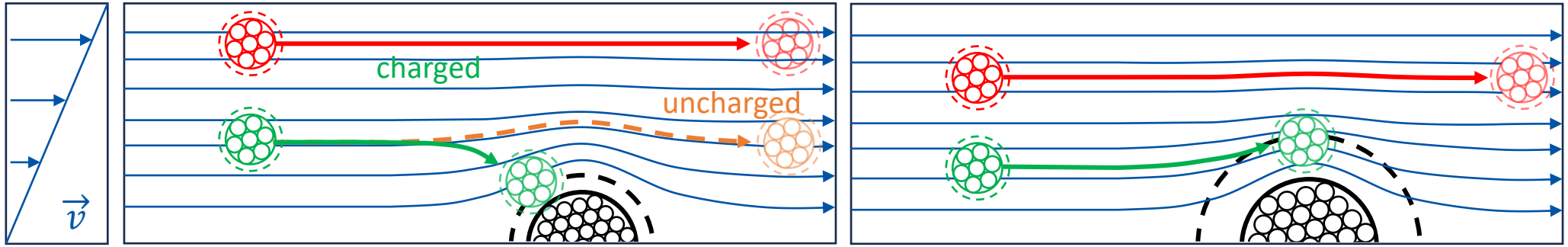
Aggregation kernel $A_{i,j}$, *the* ***shell-core concept***

$$A_{i,j} = 1.294\,\alpha_{i,j}\,\overline{G}_{\text{eff}}\,\frac{\left(d_i + d_j\right)^3}{8}\,; \qquad \alpha_{i,j} = \alpha_{i,j}^{\text{c}} + \alpha_{i,j}^{\text{p}}\,; \qquad \alpha_{i,j} \in (0,1)$$



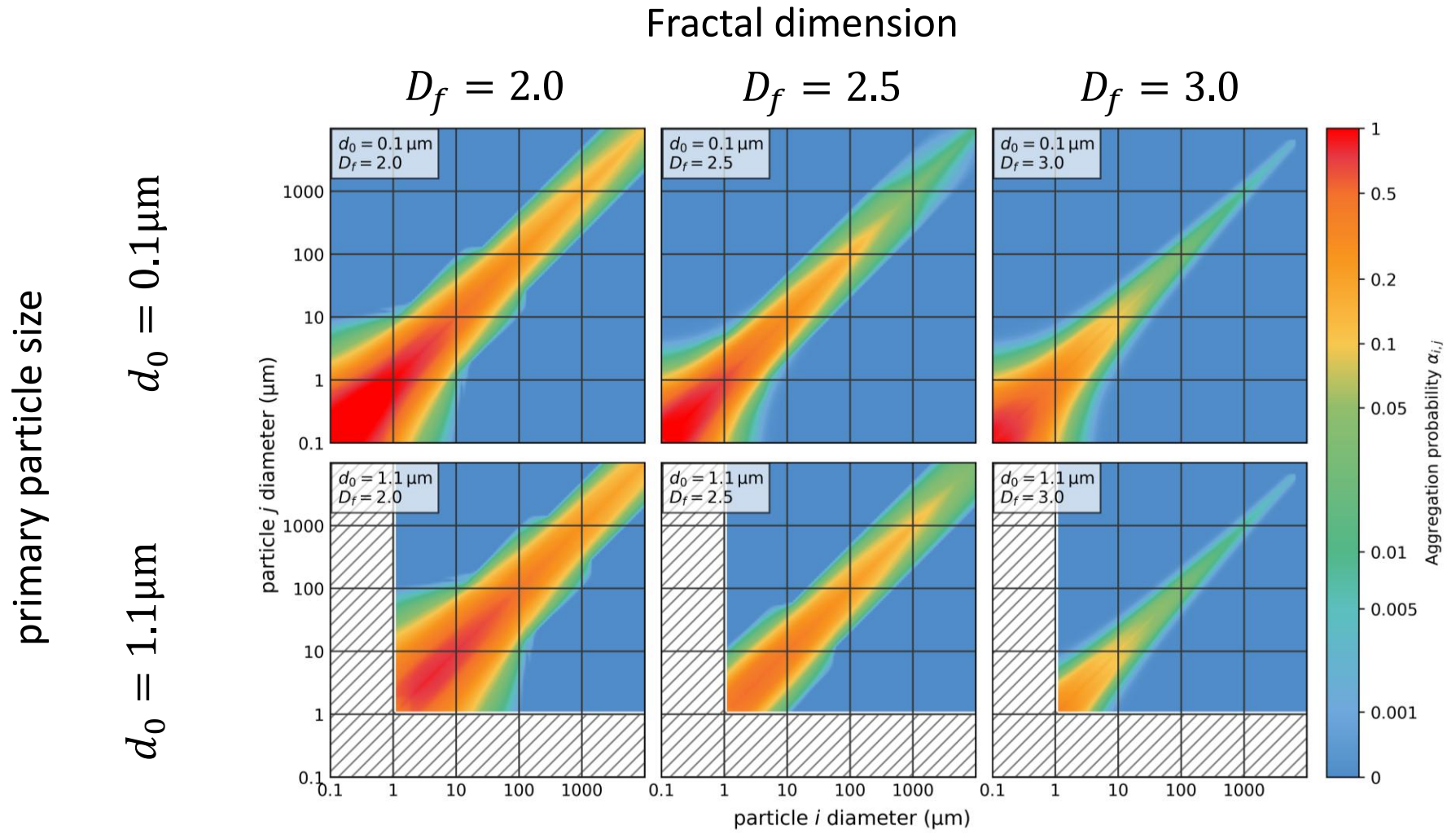
- flow around porous aggregates in simple shear flow – Adler (1981)
- implementation of shell-core concept under coagulation conditions – Kusters (1997)

a) Collision of charged cores - $\alpha_{i,j}^{\text{c}}$ b) Capture in aggregate porous shell – $\alpha_{i,j}^{\text{p}}$



Population Balance Modeling

Aggregation kernel $A_{i,j}$



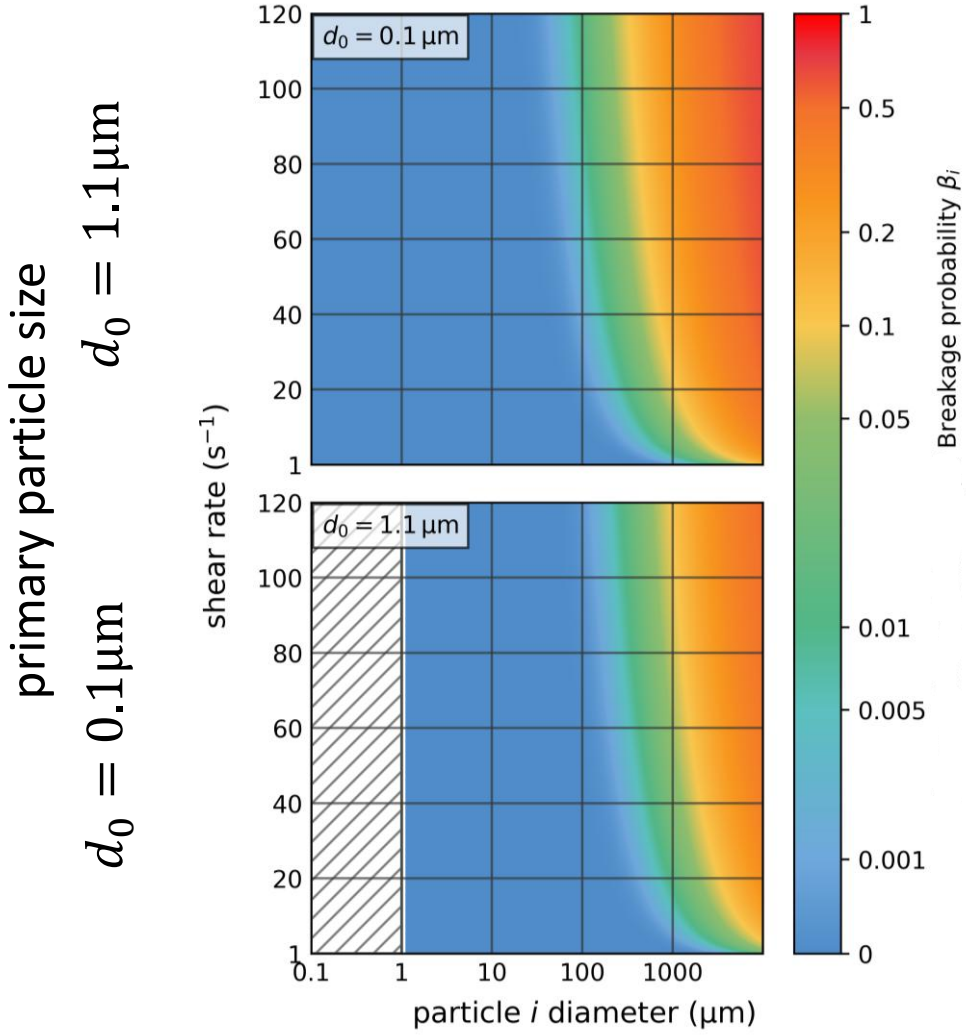
Population Balance Modeling

Breakage Kernel B_k

$$B_k = \left(\frac{4}{15\pi}\right)^{0.5} \overline{G}_{\text{eff}} \exp\left(\frac{-a}{p^b (d_k/d_0)^c}\right);$$

$$p = 1.88\rho_{\text{L}}(\varepsilon d_k)^{2/3}$$

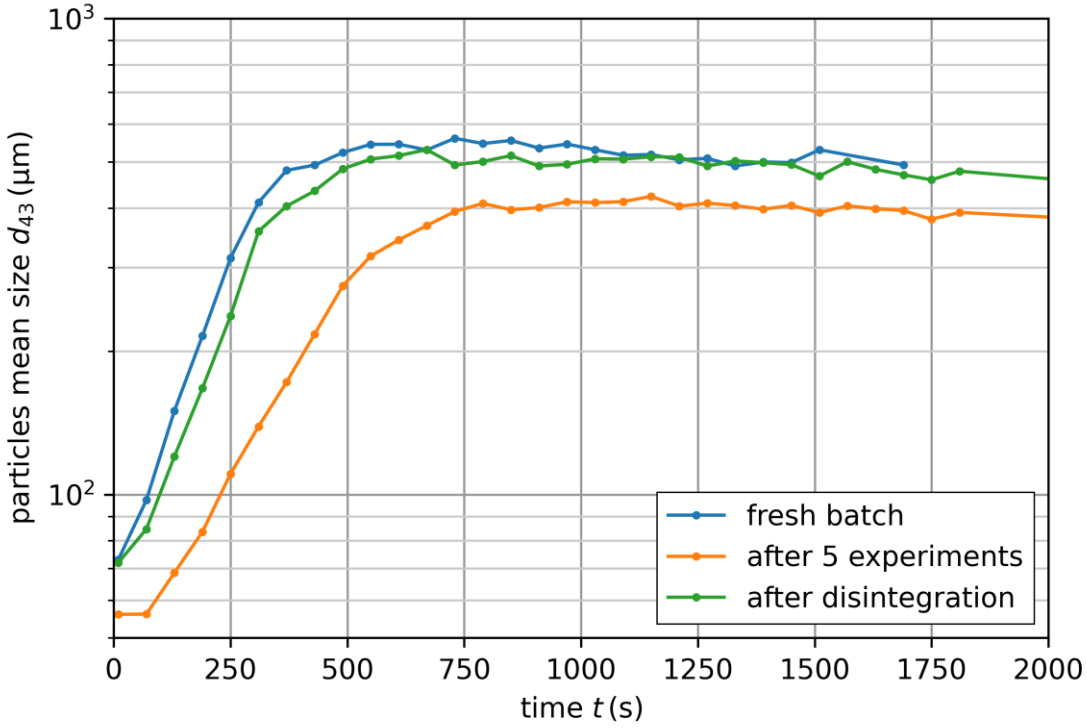
- general exponential model
- based on Kusters (1999) without fractal dimension dependence
- 3 optimized parameters a, b, c



Population Balance Modeling

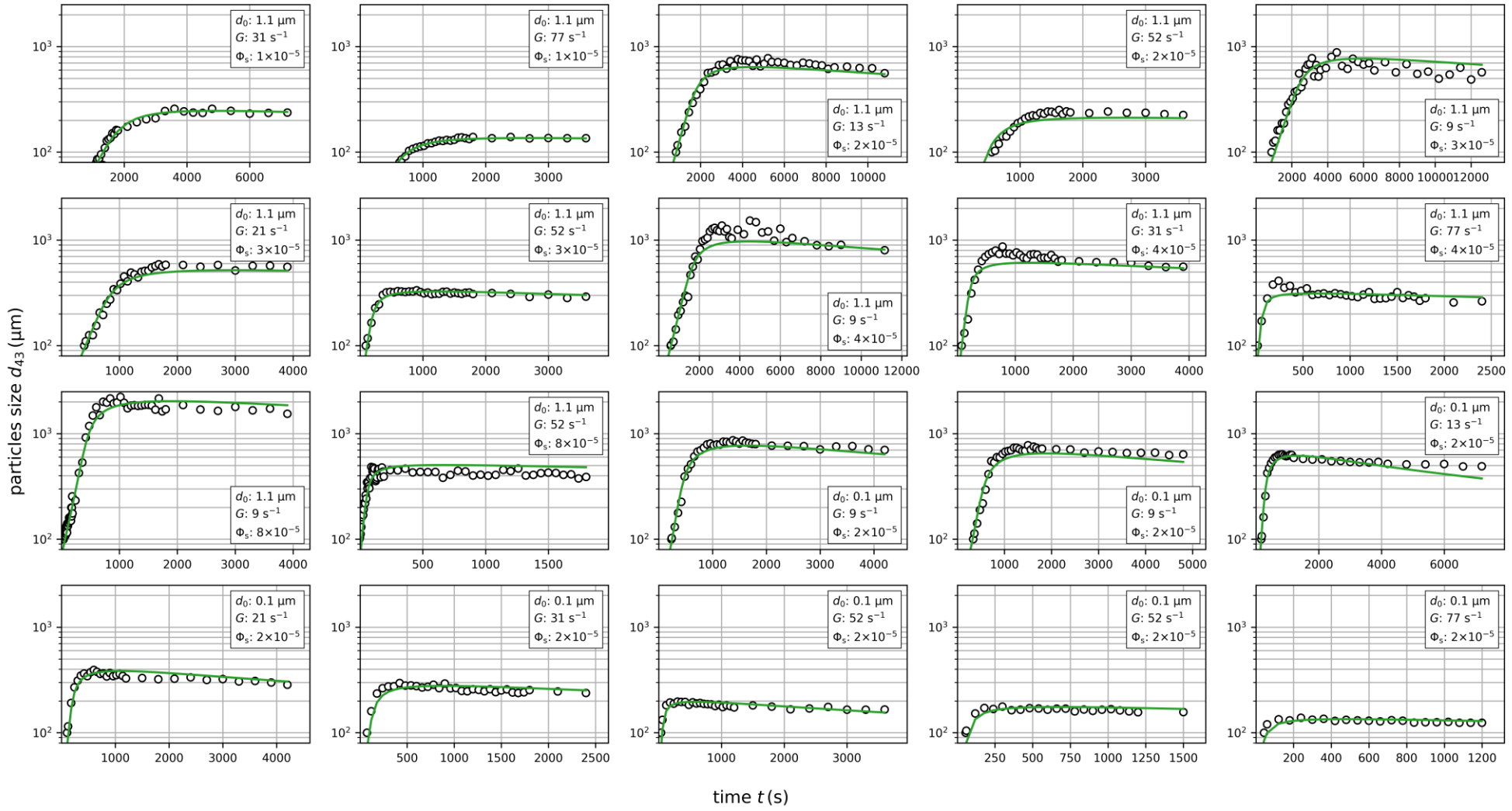
Model summary

- physics-based aggregation kernel (without optimized parameter)
- empirical breakage kernel (3 parameters $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$)
- time evolution of fractal dimension D_f
  - common optimized rate of fractal dimension evolution $\boldsymbol{\gamma}$
  - fitted initial fractal dimension for each case of $\boldsymbol{D_f}(0) = (2.1 - 2.3)$
  - common final fractal dimension $D_f^{\infty} = 3.0$
- optimized using 20 experiments, validated on the remaining 40 experiments



Population Balance Modeling

Results – $D_{4,3}$ and PSD



Population Balance Modeling

Results – $D_{4,3}$ and PSD

- model is able to catch:
  - steep initial phase of rapid growth
  - value and time required to reach the maximum $D_{4,3}$
  - decrease in size after reaching the maximum
  - evolution of size distribution
- mean and maximum error of $\overline{S} = 12\%$ and $S_{\max} = 25\%$
  - level of confidence of experimental data

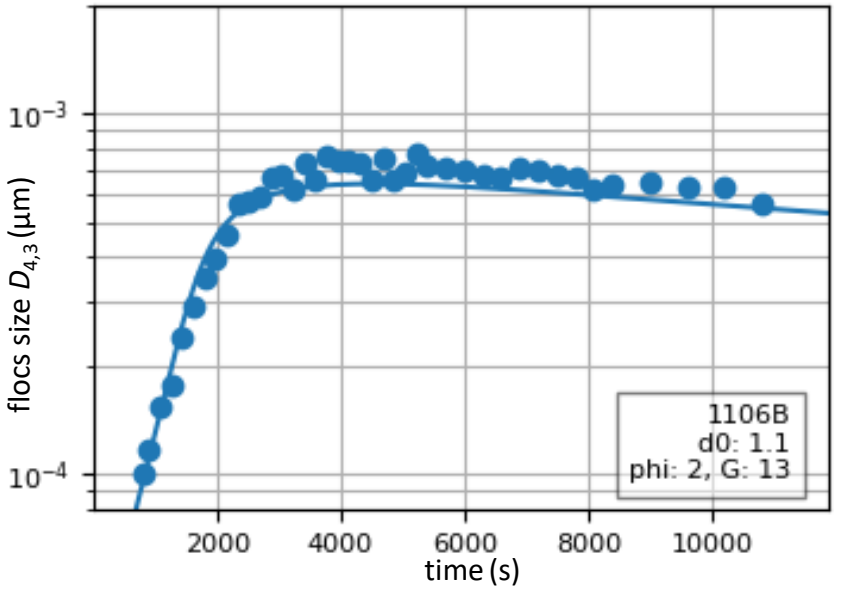
Optimized parameters of model.

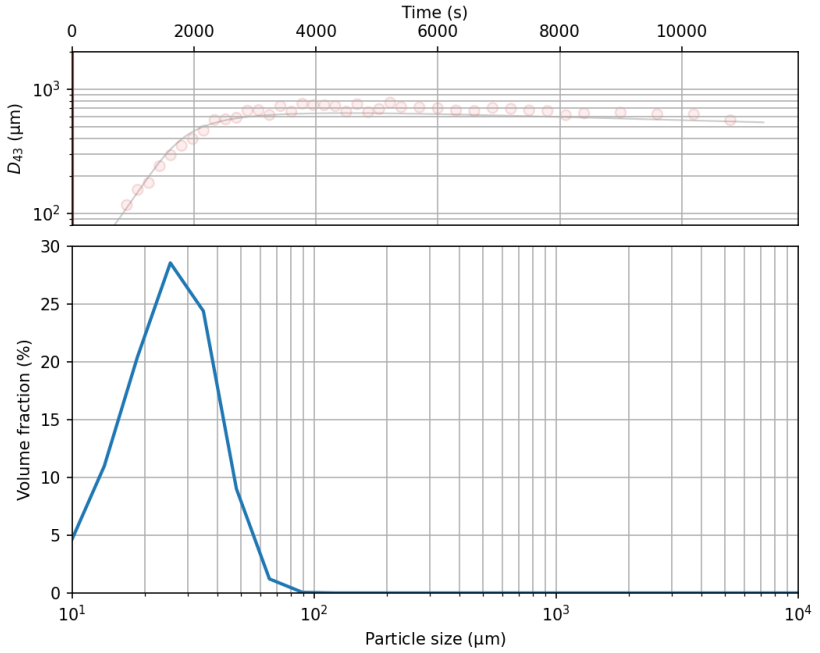
d_0 (µm)	a	b	c	γ
0.1	32.1	0.283	0.350	$2.38 \cdot 10^{-5}$
1.1	24.8			

+

Initial condition

$D_f(t = 0\ \text{s})$ for each case



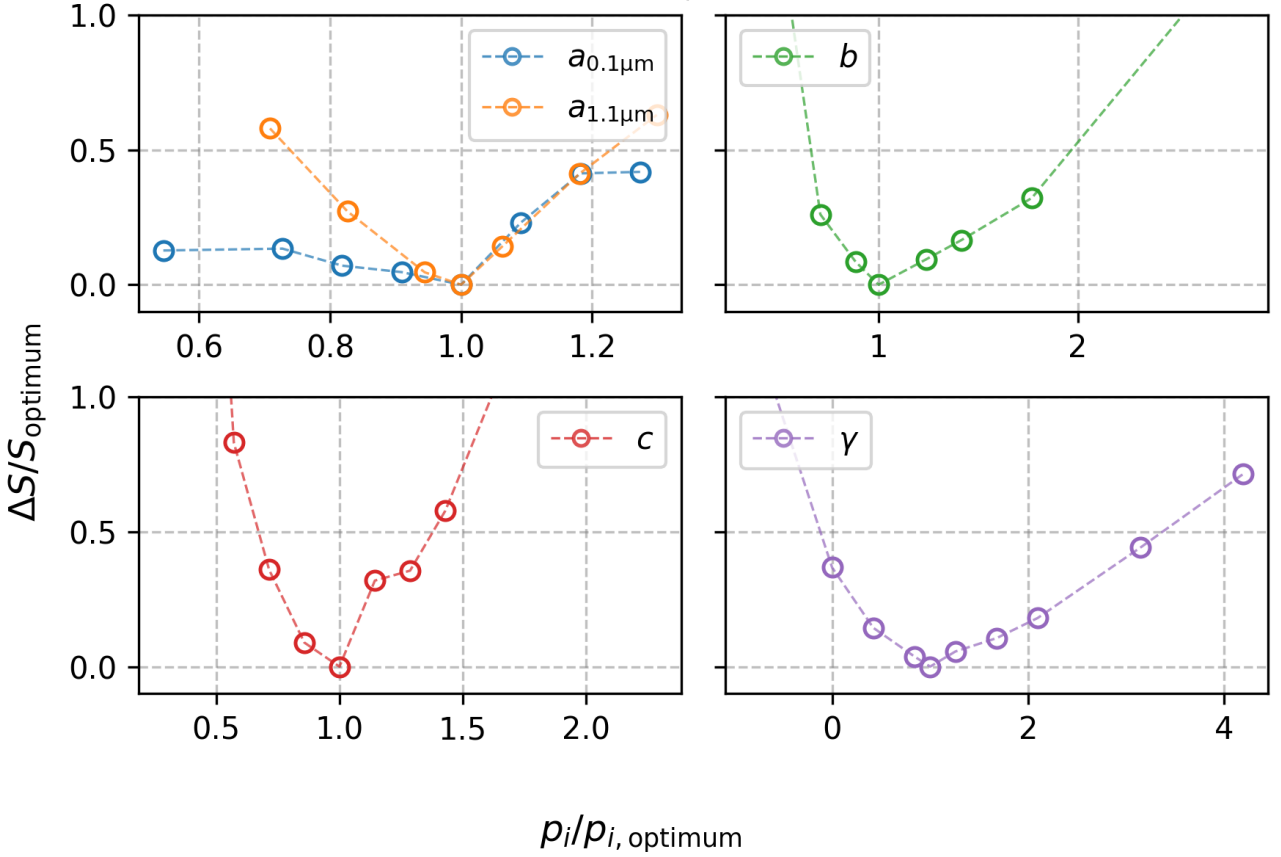


Population Balance Modeling

Results – parameters sensitivity

- fixed values of selected parameter, other ones optimized
- relatively narrow optima for ***c*** and ***b***
- relatively wide optima for $\boldsymbol{\gamma}$
- necessary development of fractal dimension ($\gamma > 0$)

$$S = \sqrt{\overline{S} S_{\max}}$$



Optimized parameters of model.

d_0 (μm)	a	b	c	γ
0.1	32.1	0.283	0.350	$2.38 \cdot 10^{-5}$
1.1	24.8			

Conclusions

Summary

- Unique set of **experimental data**; wide range of experimental conditions;
- implemented **physics-based** Adler/Kusters aggregation kernel;
- successfully fitted experimental data with mean error of 12%.

Future outlook

- PBM model transfer to flocculation with nature water matrices and coagulant;
- couple PBM model with local hydrodynamic conditions by means of CFD.

Thank you for your attention.

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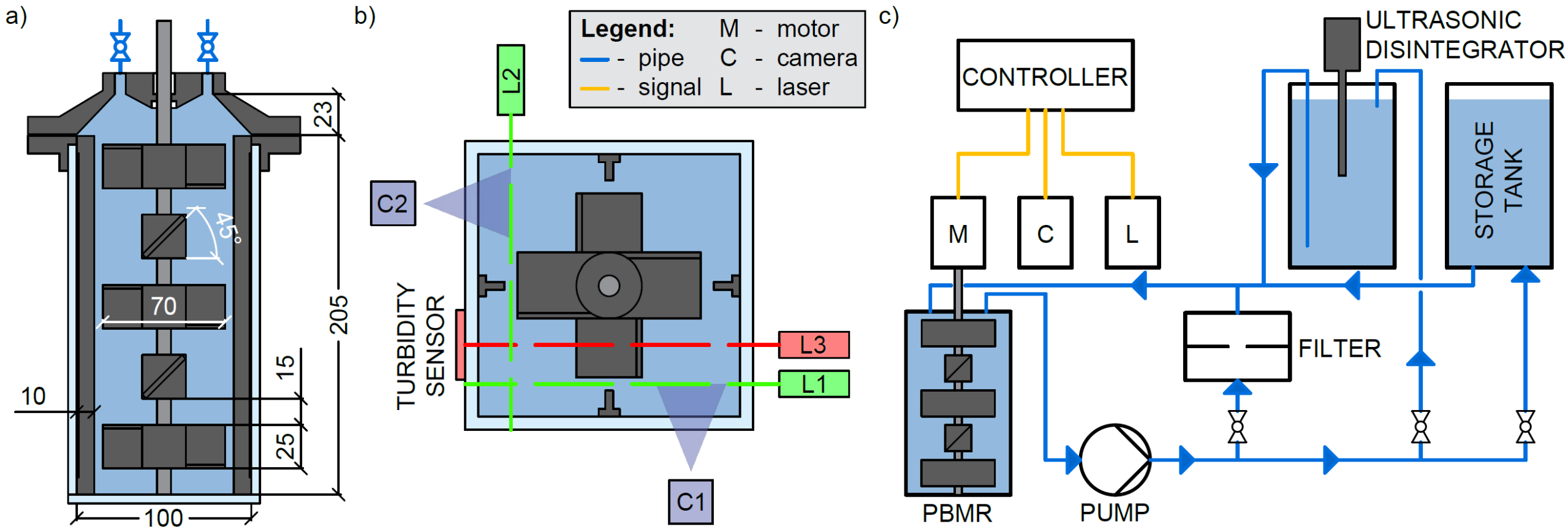
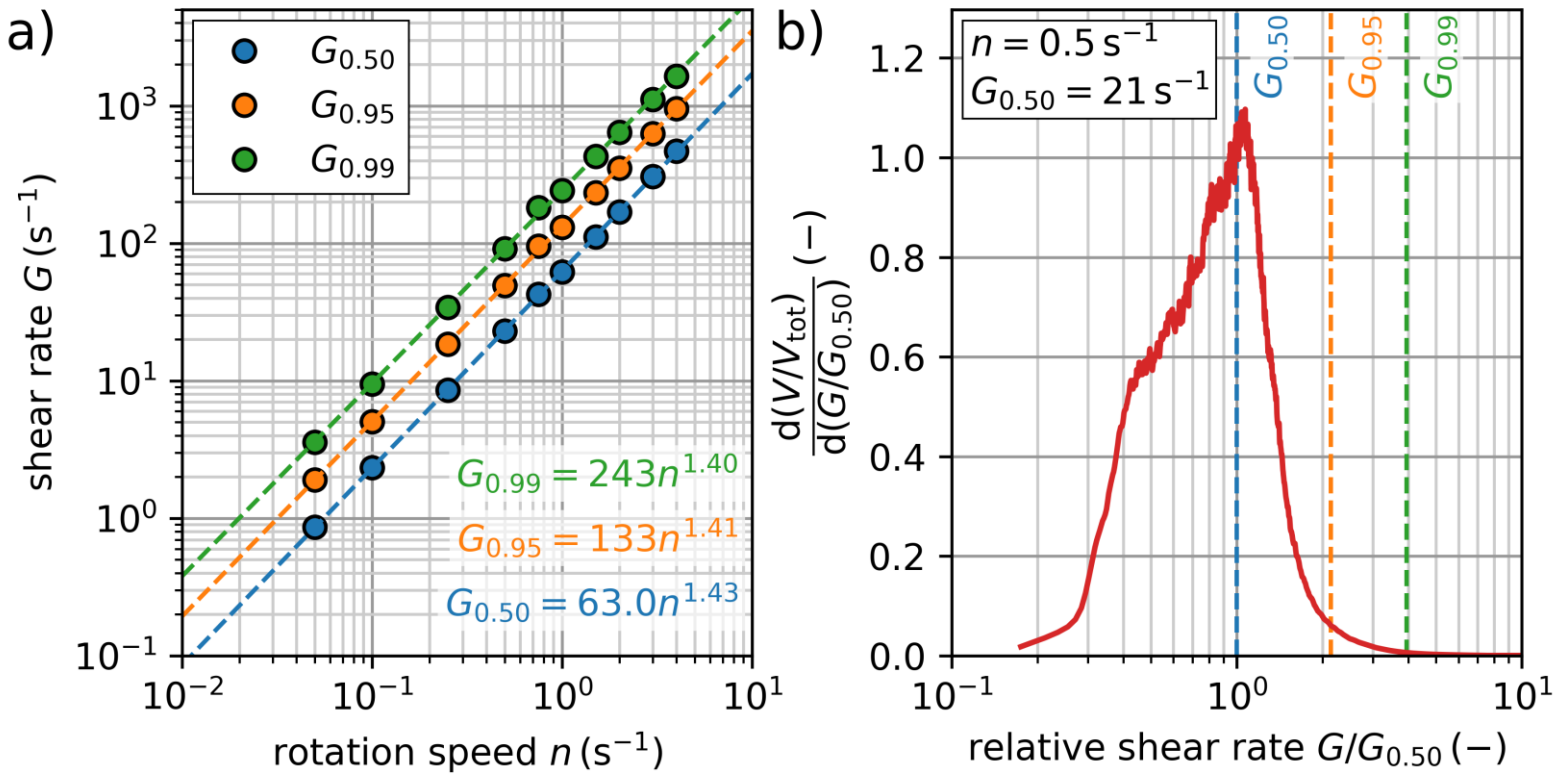
Supporting materials

Experimental



Supporting materials

Experimental



Supporting materials

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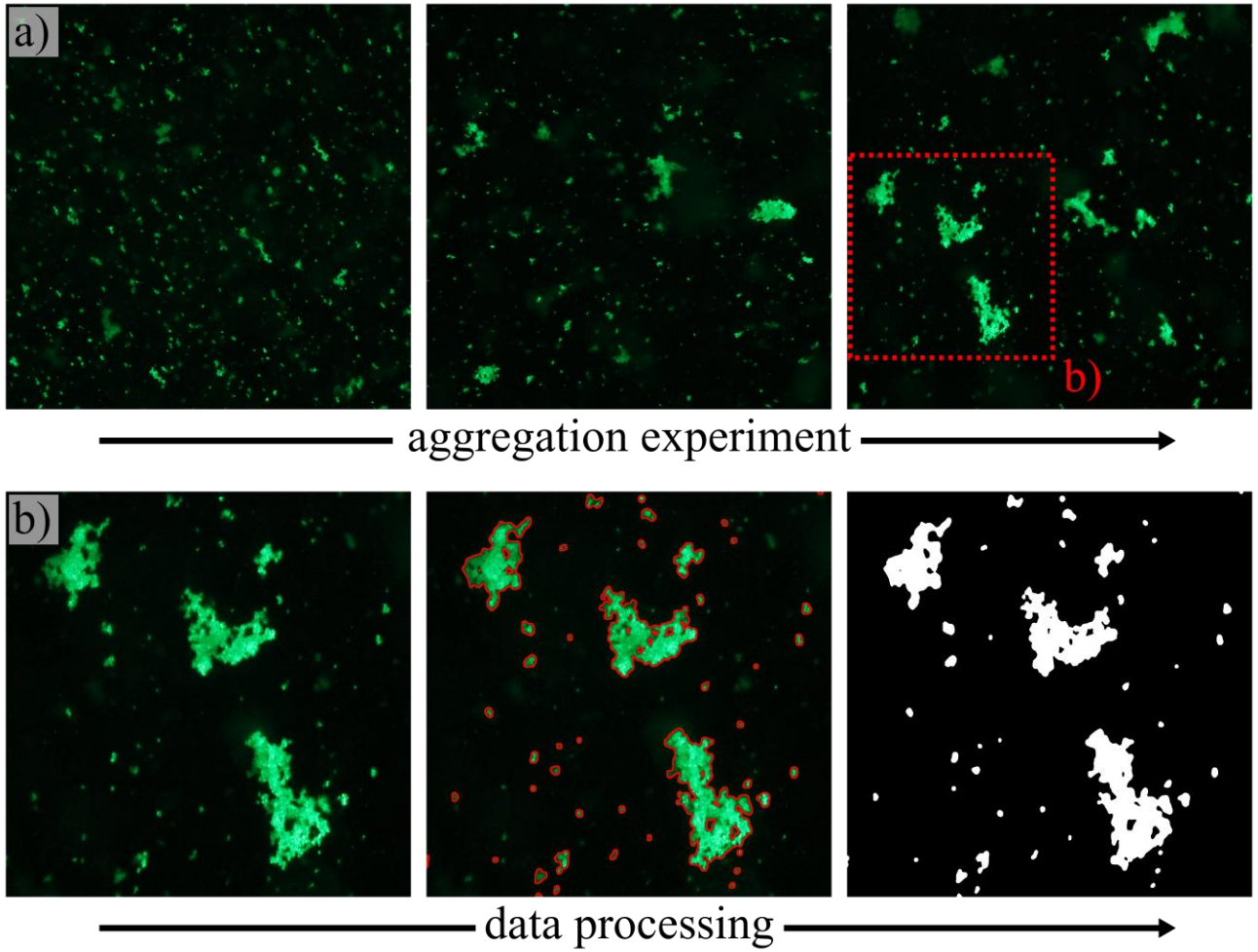

Supporting materials

Effective mean velocity gradient – $\overline{G}_{\mathrm{eff}}$

$$\overline{G}_{\mathrm{eff}} = \begin{cases} \overline{G}, & L \lesssim 6\eta_{\mathrm{K}}, \\ 1.83\overline{G}^{5/6}\nu_{\mathrm{L}}^{1/6}L^{-1/3}, & 6\eta_{\mathrm{K}} < L \lesssim 25\eta_{\mathrm{K}}, \\ 5.33\overline{G}^{2/3}\nu_{\mathrm{L}}^{1/3}L^{-2/3}, & L > 25\eta_{\mathrm{K}}. \end{cases}$$

$$L = \begin{cases} r_i + r_j, & \text{aggregation}, \\ r_k, & \text{breakage}. \end{cases}$$

Supporting materials

Batch history

Supporting materials

PBM protocol

