

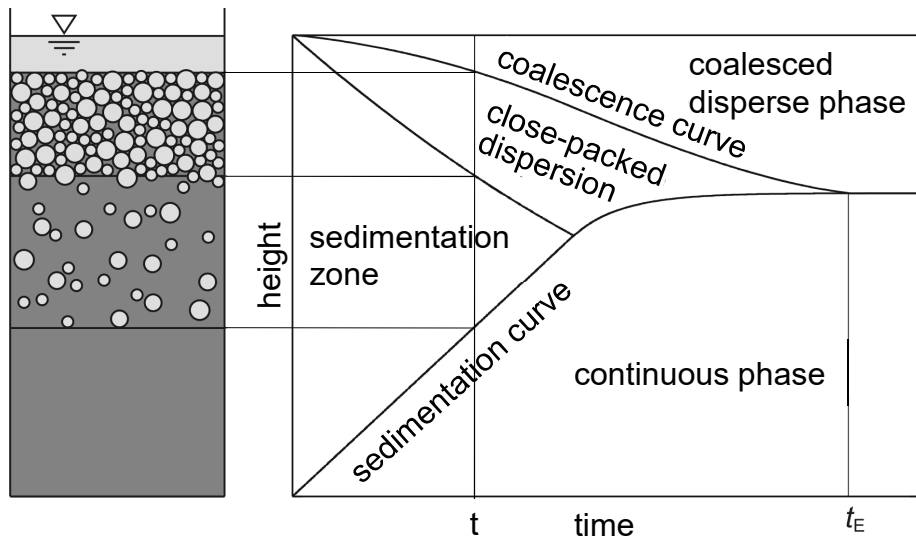
International Solvent Extraction Conference (ISEC 2022)
Göteborg, Sweden, Sept. 26 to 30, 2022

Detailed Drop-Based Simulation of Settling Behavior

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general settler concept

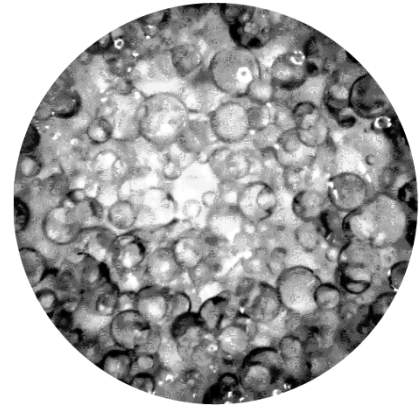
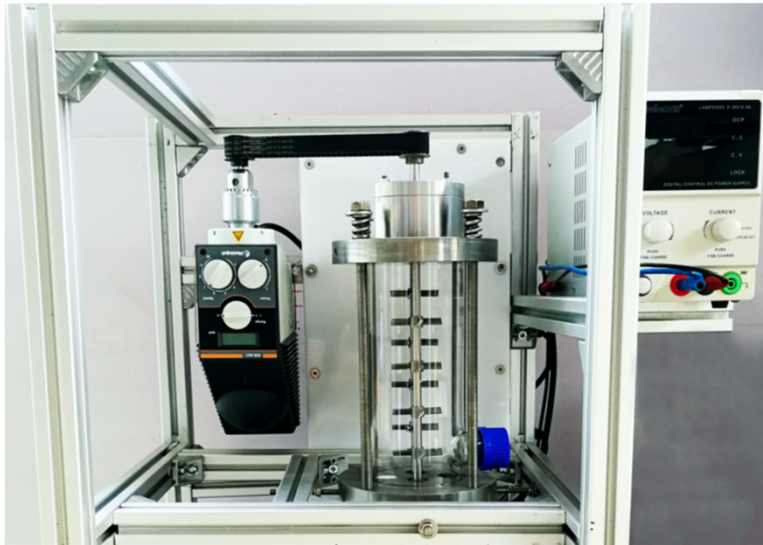


e.g.: Henschke, Schlieper, Pfennig, 2002: Determination of a coalescence parameter from batch-settling experiments. Chem. Eng. J. 85, 369-378.

2

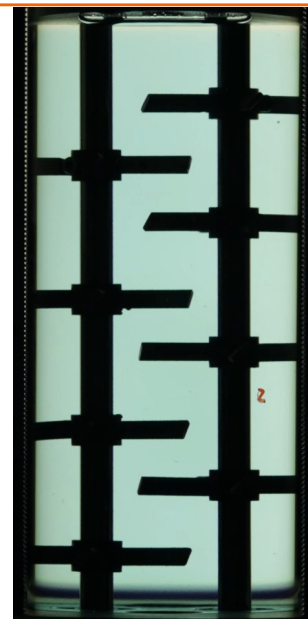


settling cell with SOPAT probe

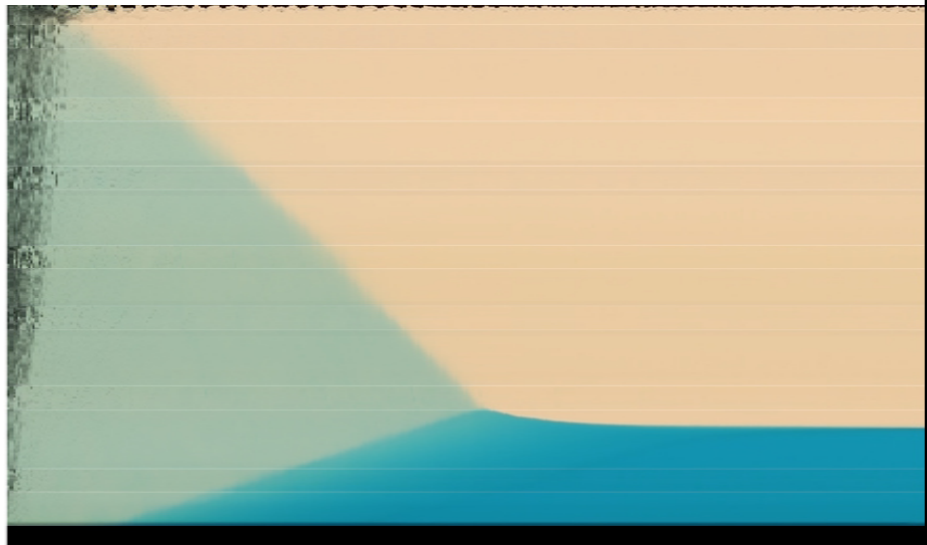


iso-optical system

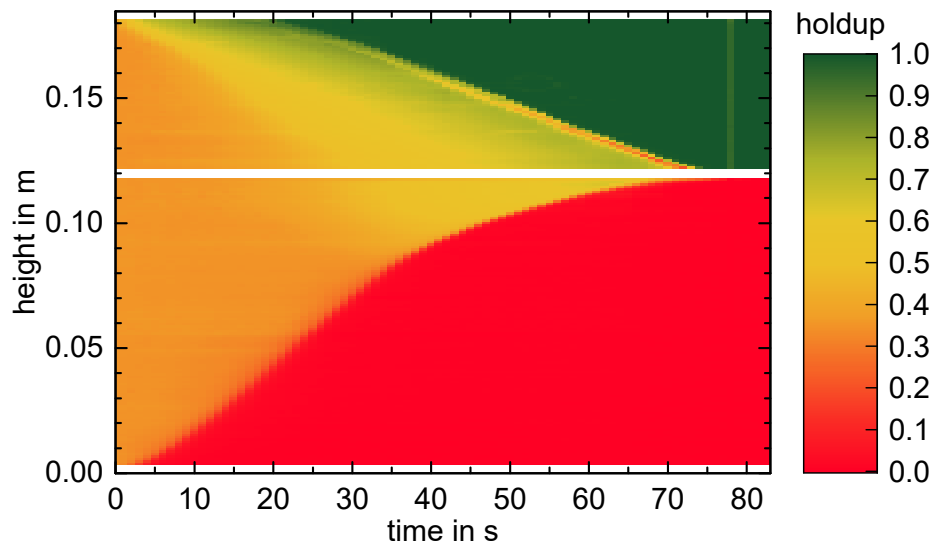
- water + ethylene glycol + hexane
- identical refractive index of phases
 - no refraction at interface
 - transparent dispersion



iso-optical system



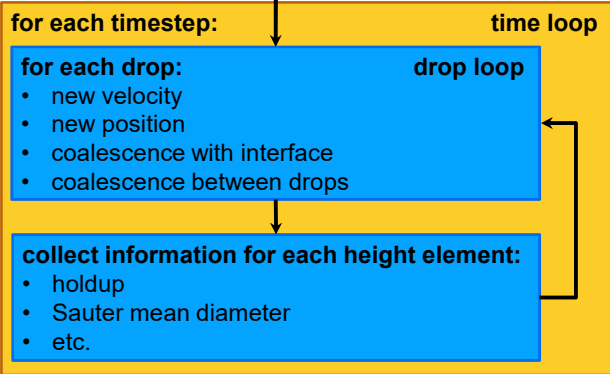
experimental holdup, initial holdup: 35 % organic



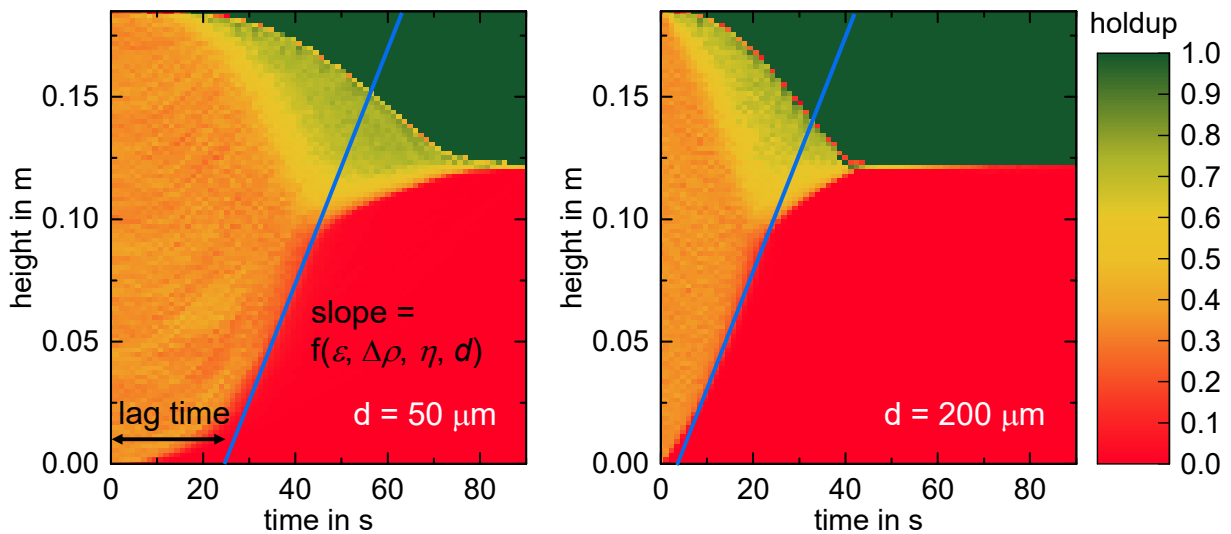
ReDrop: drop-based modeling

definition of system:

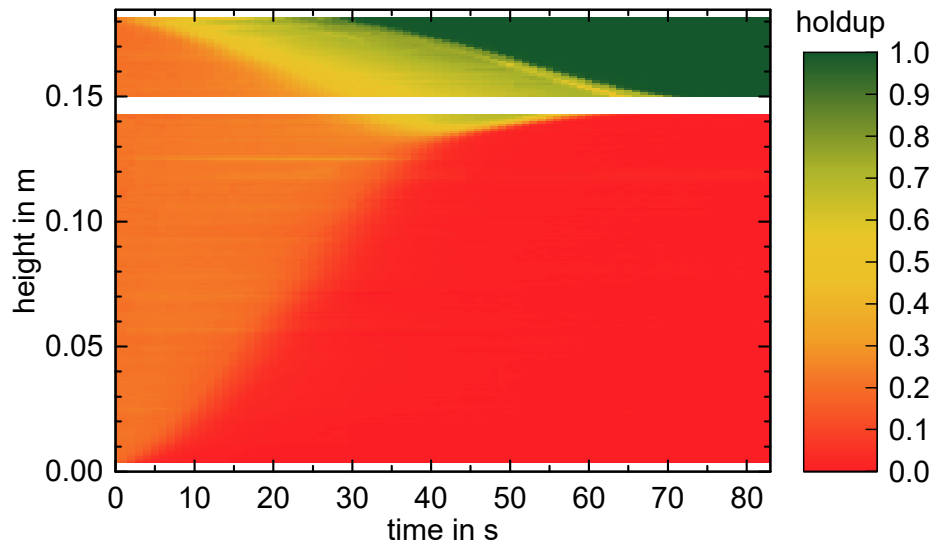
- material properties
- process variables
- simulation parameters
- set up arrays and system



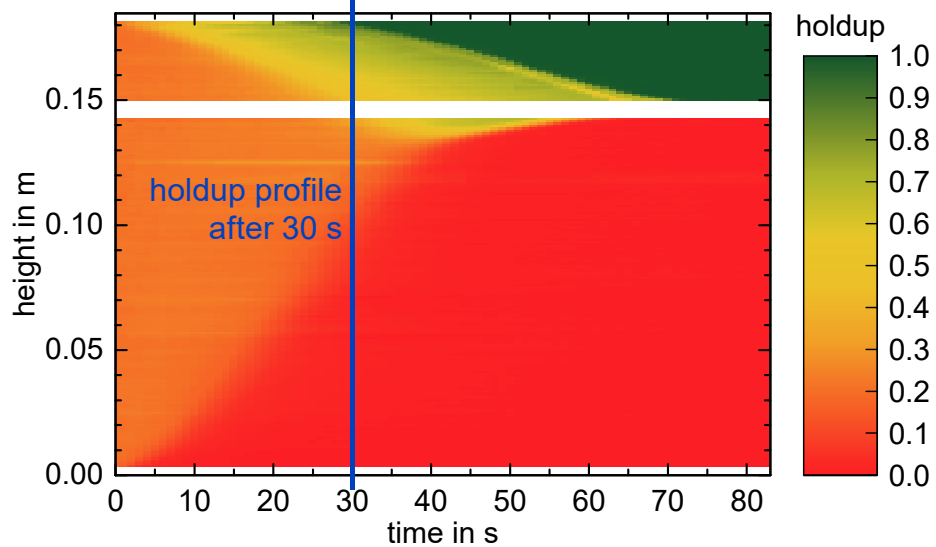
lag time & characteristic drop diameter



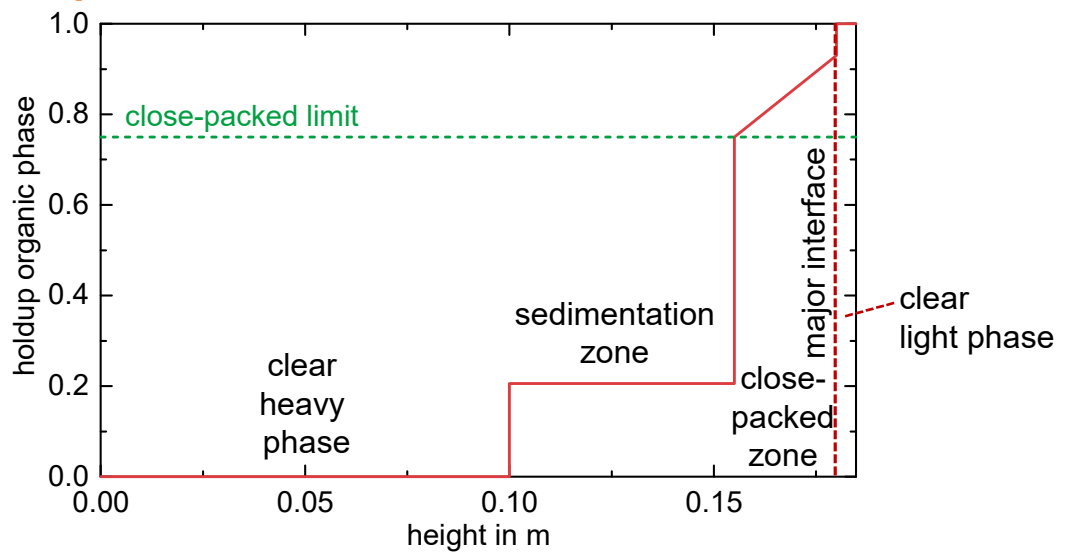
experimental holdup, initial holdup: 20.5 % organic



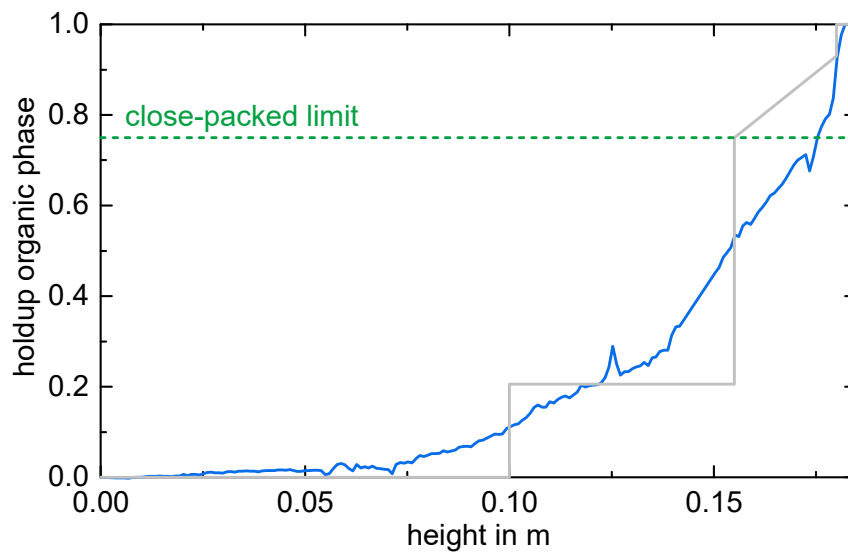
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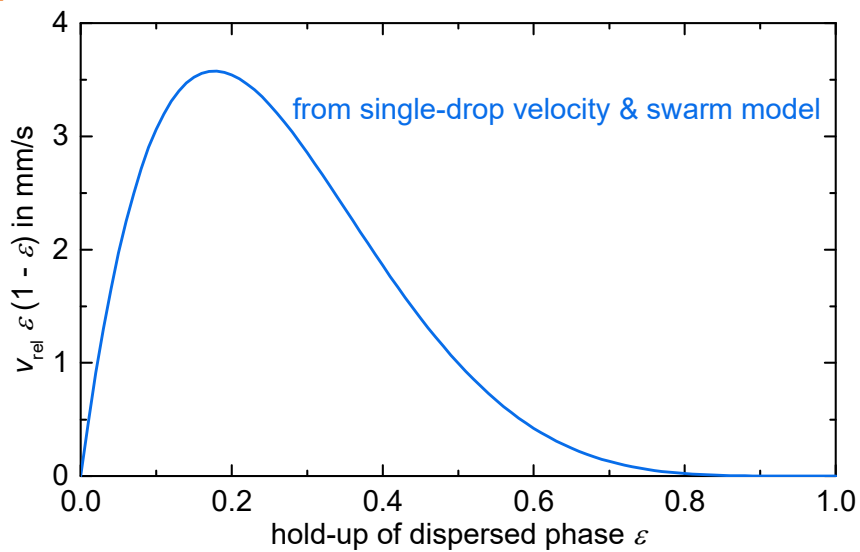
what we expect



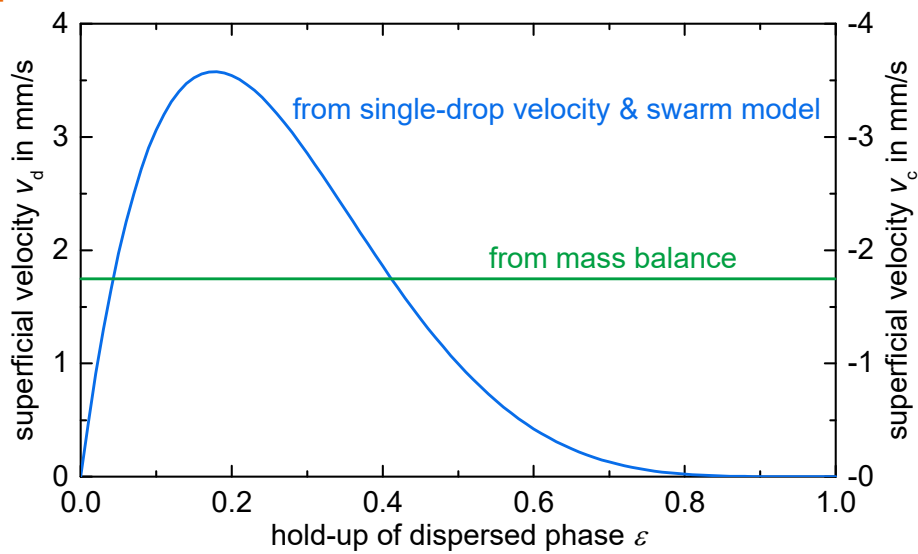
what we find



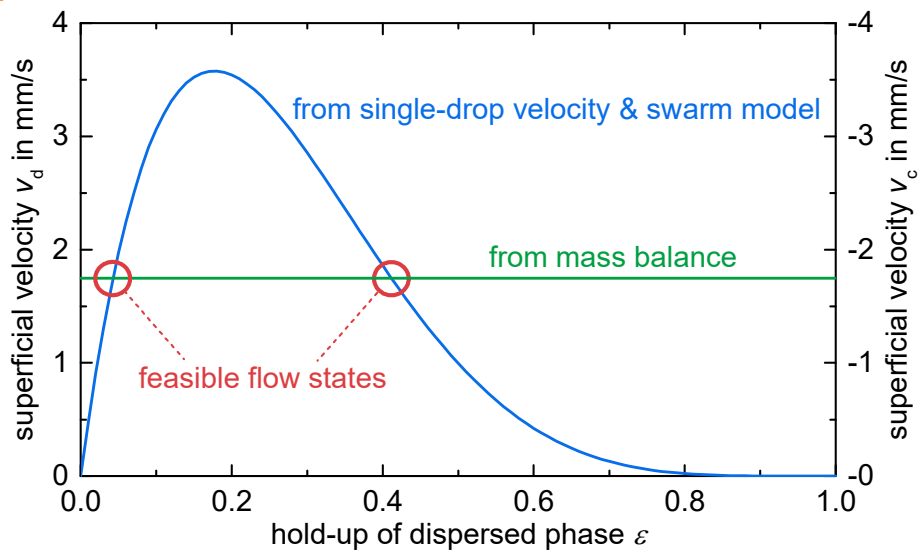
Wallis plot



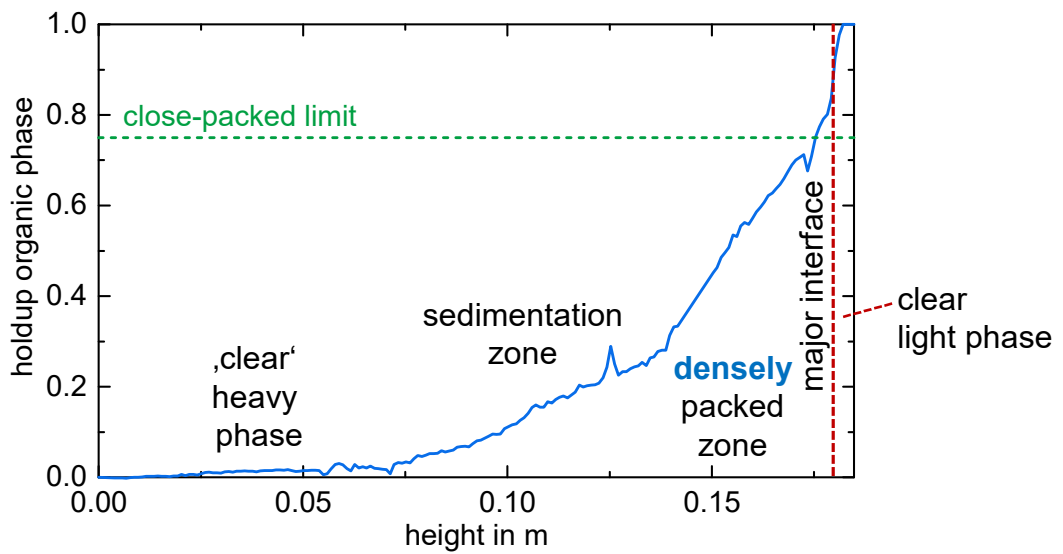
Wallis plot



Wallis plot

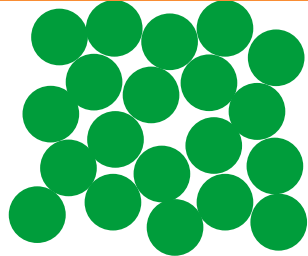


what we find



at the interface

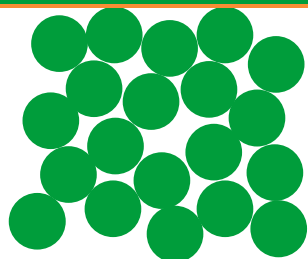
interface



before coalescence

at the interface

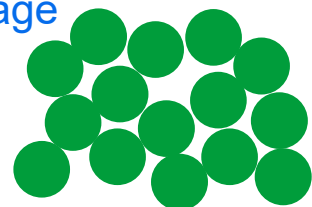
interface



before coalescence

interface

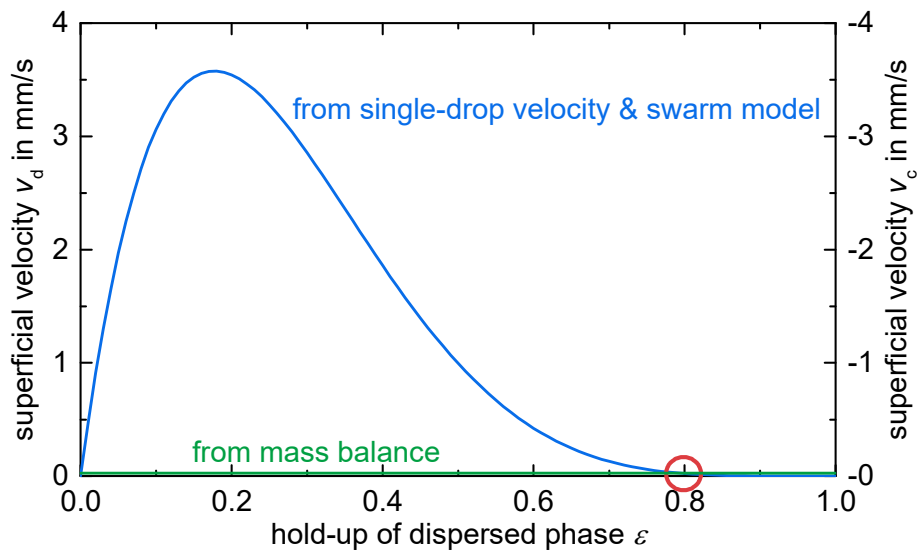
voidage



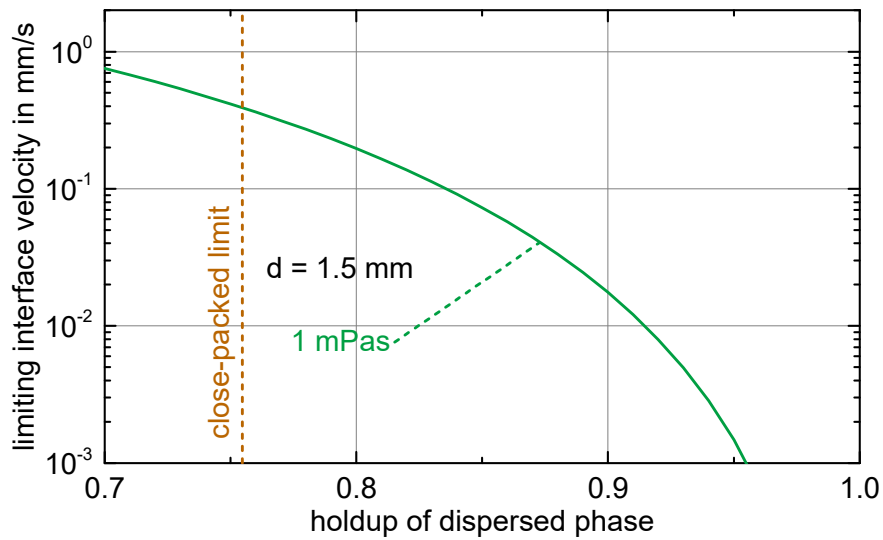
after coalescence

dispersed phase
continuous phase

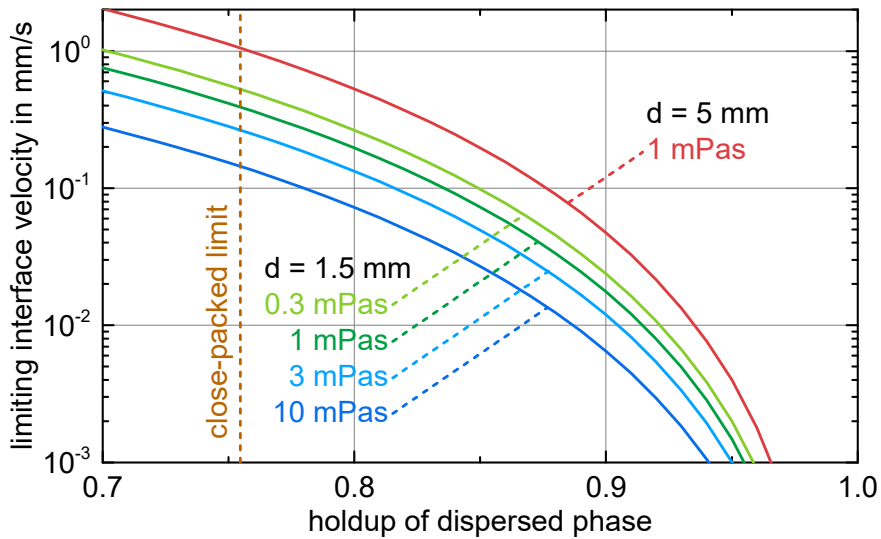
flowrate close to interface



is this a general effect?



is this a general effect?



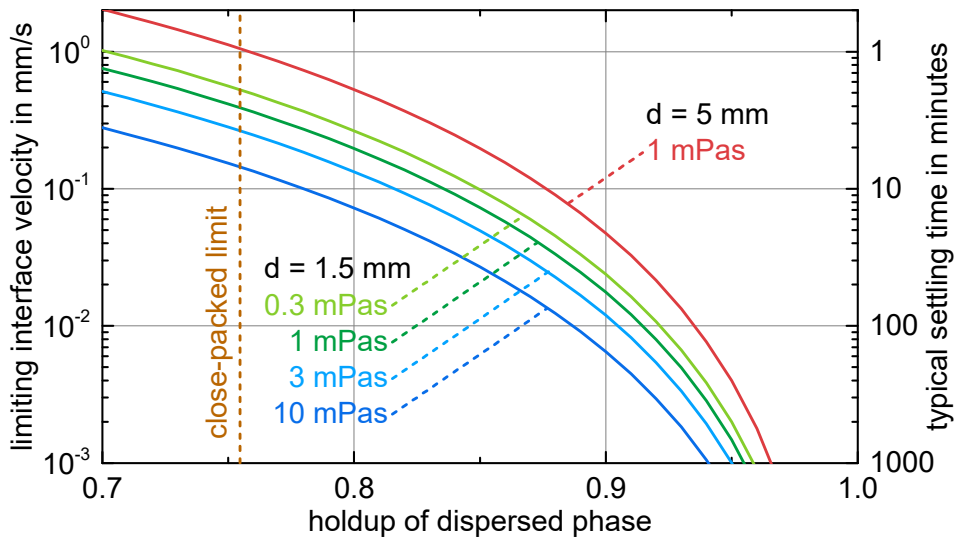
$\Delta\rho = 400 \text{ kg/m}^3$

model: Henschke, Waheed, Pfennig, 2000 & Richardson, Zaki, 1954

21



is this a general effect?



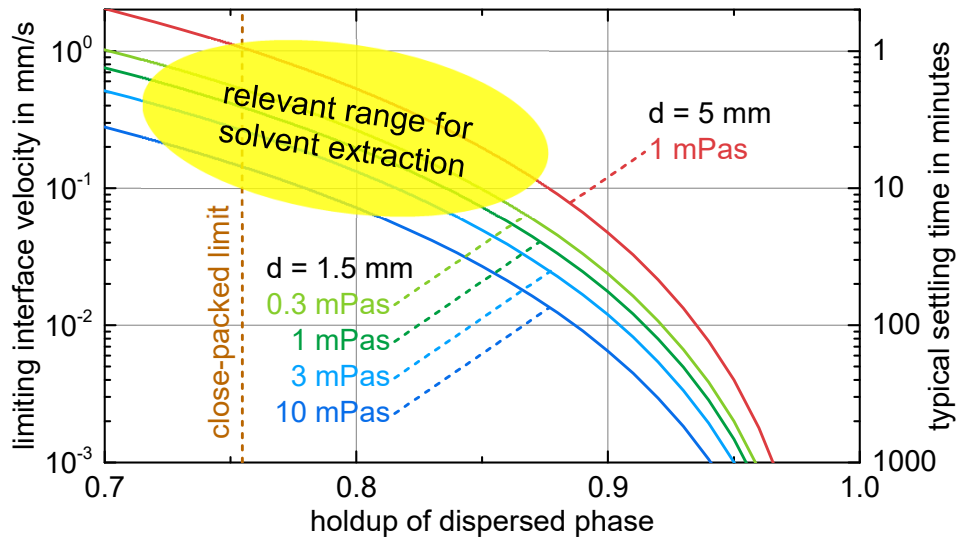
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is this a general effect?



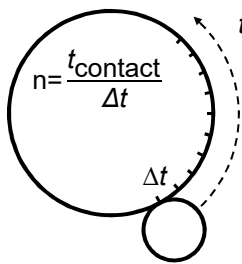
coalescence probability

Coulaloglou & Tavlarides:
$$p_C = \exp\left(-\frac{t_{\text{coalescence}}}{t_{\text{contact}}}\right)$$

coalescence probability

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but:



$$p_{\text{non-c}, n\Delta t} = p_{\text{non-c}, \Delta t}^n$$

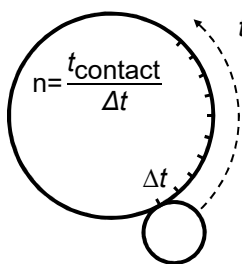
$$p_{\text{non-c}, \Delta t} = \exp\left(-\frac{\Delta t}{t_{\text{coalescence}}}\right)$$

$$p_{\text{non-c}, n\Delta t} = \exp\left(-\frac{n\Delta t}{t_{\text{coalescence}}}\right) = \exp\left(-\frac{t_{\text{contact}}}{t_{\text{coalescence}}}\right)$$

coalescence probability

~~Coulaloglou & Tavlarides: $p_c = \exp\left(-\frac{t_{\text{coalescence}}}{t_{\text{contact}}}\right)$~~

but:



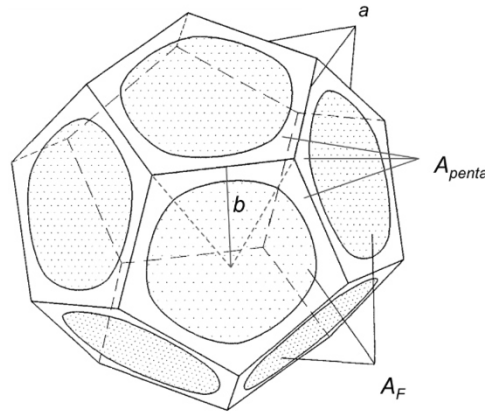
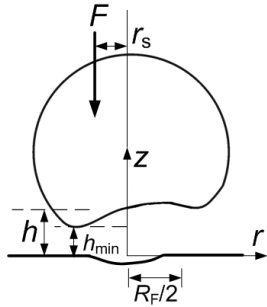
$$p_{\text{non-c}, n\Delta t} = p_{\text{non-c}, \Delta t}^n$$

$$p_{\text{non-c}, \Delta t} = \exp\left(-\frac{\Delta t}{t_{\text{coalescence}}}\right)$$

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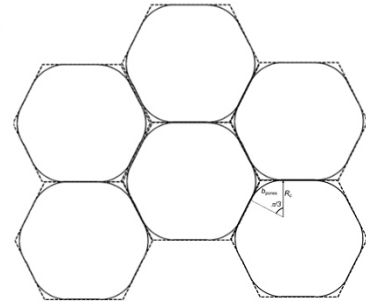
⇒ correct: $p_c = 1 - \exp\left(-\frac{t_{\text{contact}}}{t_{\text{coalescence}}}\right)$

coalescence: polyhedron & asymmetric dimple model

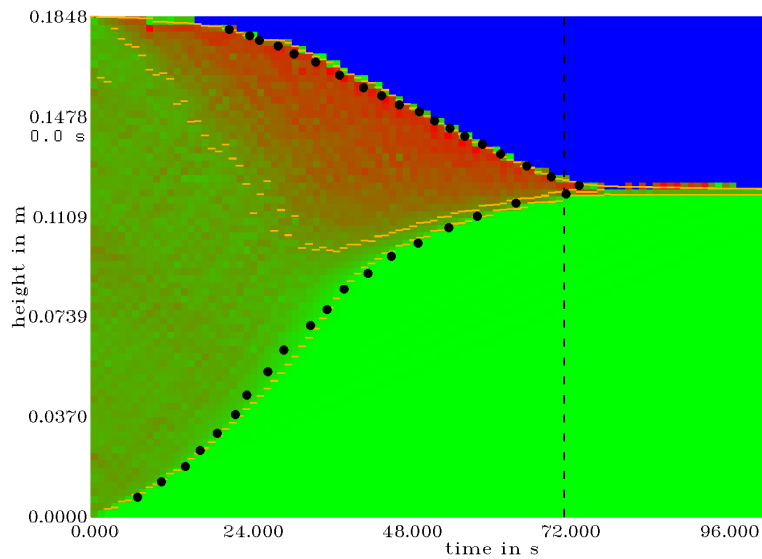


$$t_{\text{coalescence}} \sim \frac{6\pi^2 \mu R_F R_a^{3/2}}{F_{\text{driving}} r_s^* \sqrt{h_{\text{critical}}}}$$

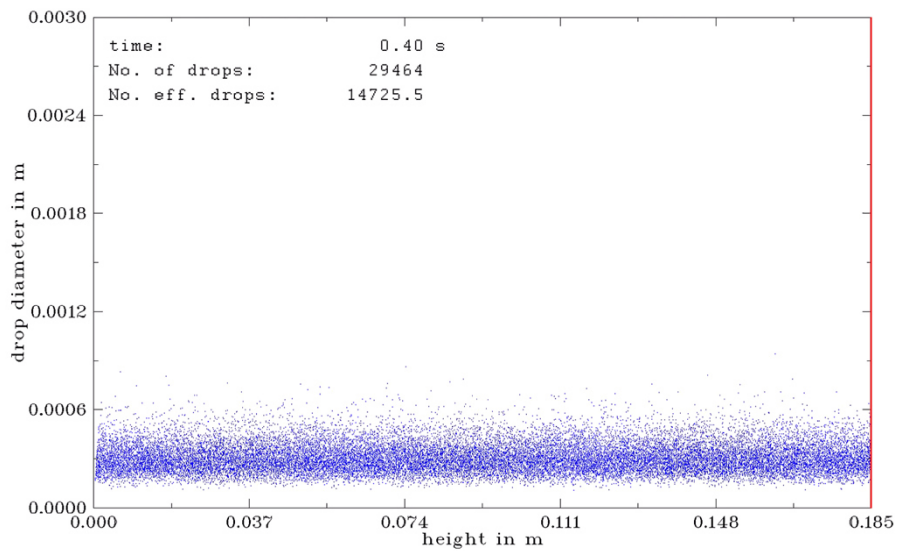
$$F_{\text{driving}} = F_{\text{Young-Laplace}} = \frac{2\pi R_F^2 \sigma}{R}$$



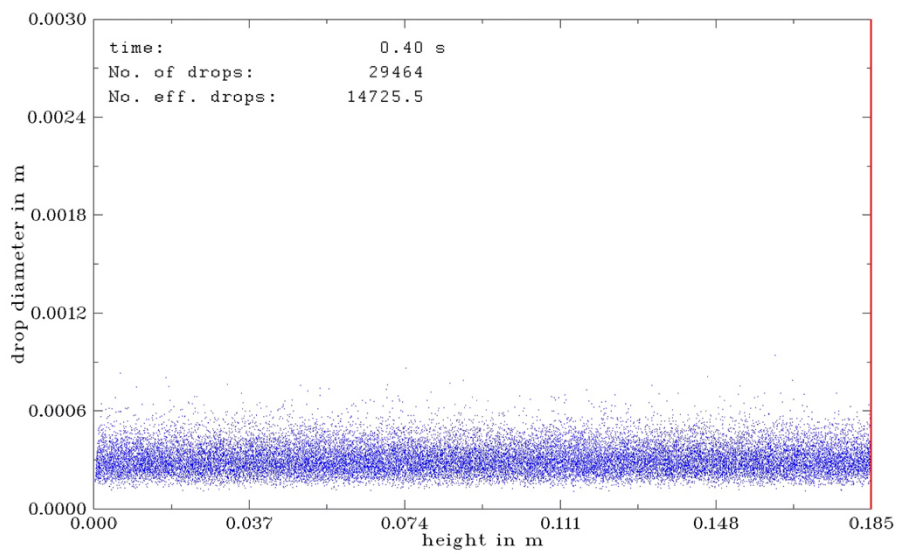
drop-based simulation results



drop-based simulation results



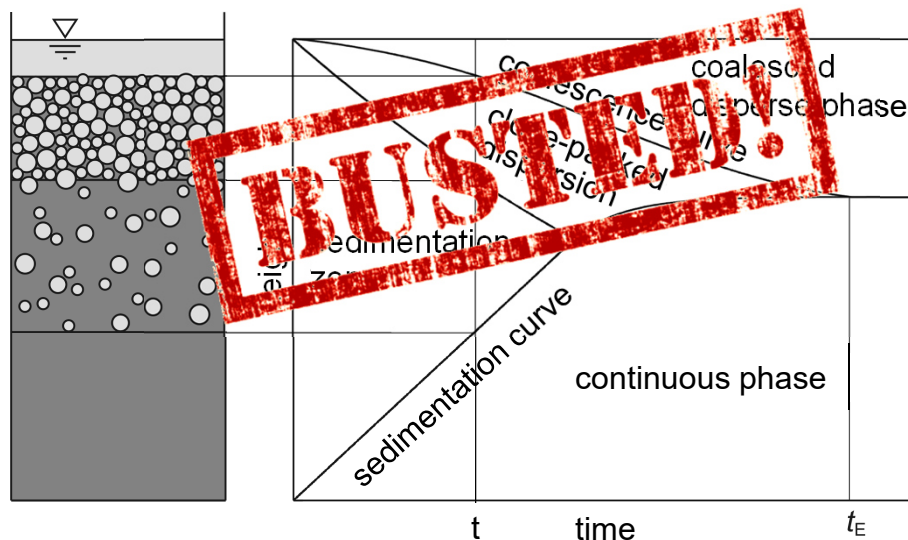
drop-based simulation results



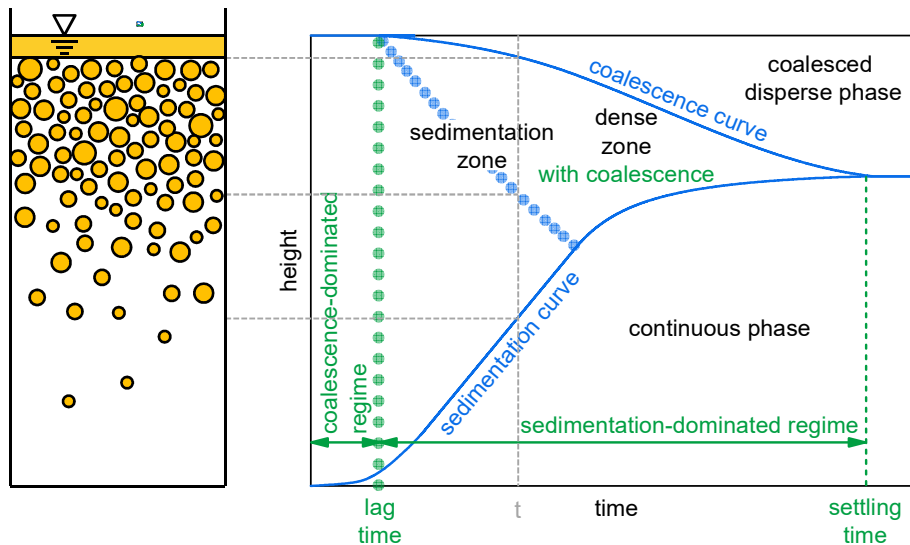
conclusions

- **lag time**: small drops, hardly sediment but coalesce \Rightarrow **polydispersity**
- **densely packed zone** \Rightarrow **velocity** of drop swarm **up to high holdup**
- close-packed zone:
 - occurs at most in small regions
 - drops don't press on each other and on interface
- modeling, simulation: ReDrop (representative drops)
 - drop sedimentation: polydisperse swarm up to high holdup
 - coalescence: Henschke polyhedron & asymmetric dimple model & correct coalescence probability

old general settler concept



new general settler concept



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