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## Introduction

High viscosity of bio-based materials induces difficulties to design technical settlers due to wide drop-size distribution, e.g. quantitative prediction of the remaining fraction of fine drops found at the settler outlet.

In parallel, trace components influence the coalescence and thus the settling behavior. It varies with the ions type and with their concentration making settling quite unpredictable. Usually, settling experiments are conducted in a so-called settling cell. From the experiment, the system can be characterized [1,2].

A numerical tool, based on the ReDrop concept (Representative Drops) [1], was developed in order to simulate the separation of liquid-liquid dispersion and thus to improve the design of continuous settler. Sedimentation and coalescence are evaluated for a sufficiently large ensemble of representative individual drops at each time step.

The coalescence modeling is a major challenge in these simulations due to trace components influence and is investigated in detail.

## ReDrop concept

### definition of the system

- material properties: density, viscosity, etc.
- simulation parameters: initial hold up, drop-size distribution, time step, coalescence parameter, etc.

local holdup evaluated for each height element

time loop

- drop loop
- individual velocity via sedimentation model
  - vertical position of each drop
  - coalescence frequency between drops following each other

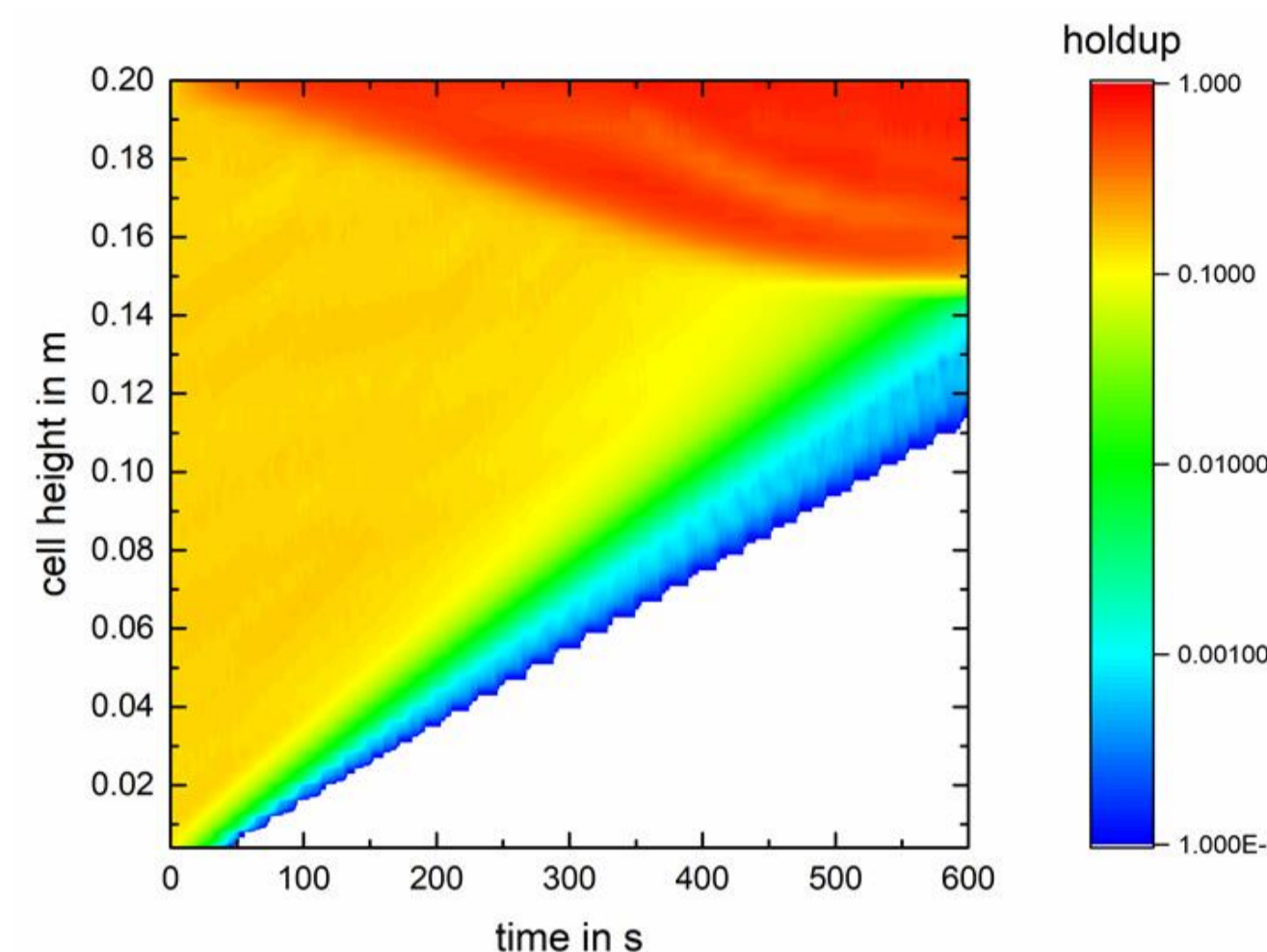


Figure 1. ReDrop simulation

- horizontal position of drops is assumed to be randomly distributed, special care is taken to evaluate contact probability to quantify correctly the coalescence
- the initial drop-size distribution can be chosen according to various distribution functions
- gas bubbles and solid particles can be accounted for as additional dispersed phases

## Coalescence model

- fluid-dynamic dependent variables have to be characterized once for a dedicated equipment
- the coalescence time depends on the material properties: solvent, salt concentration, trace components

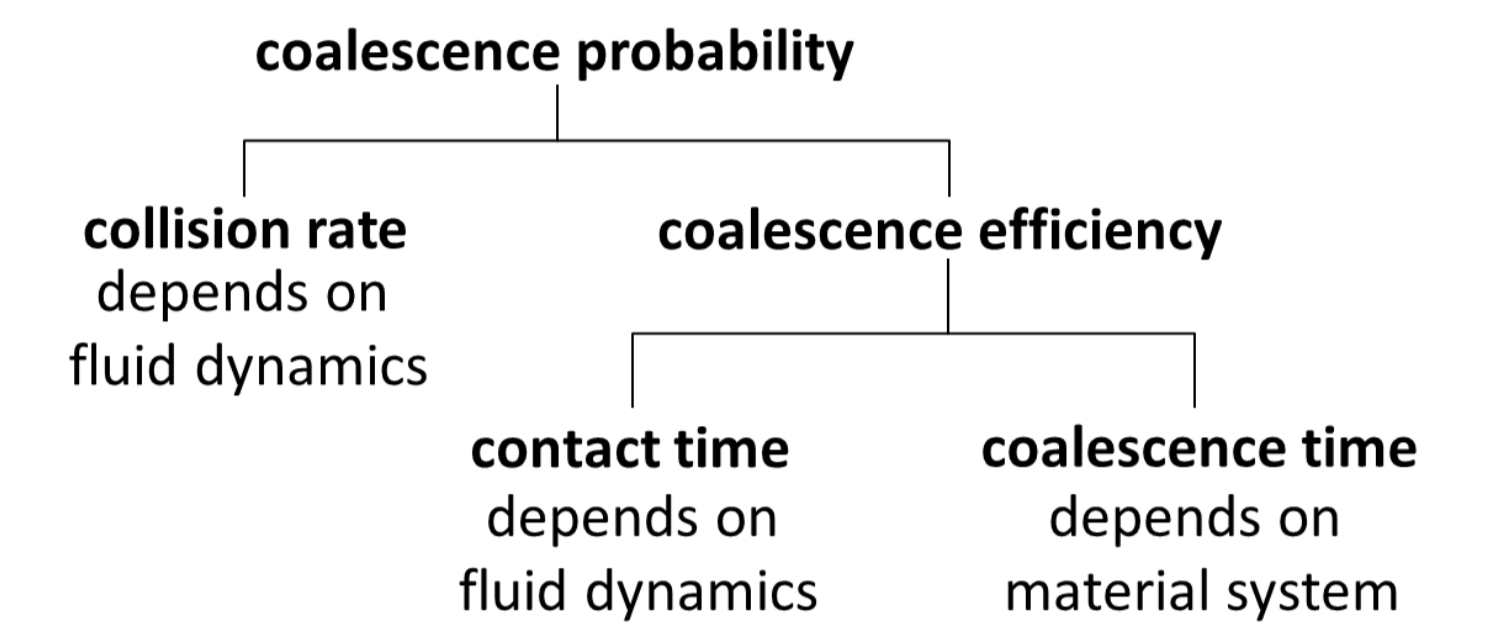


Figure 2. The coalescence model [3]

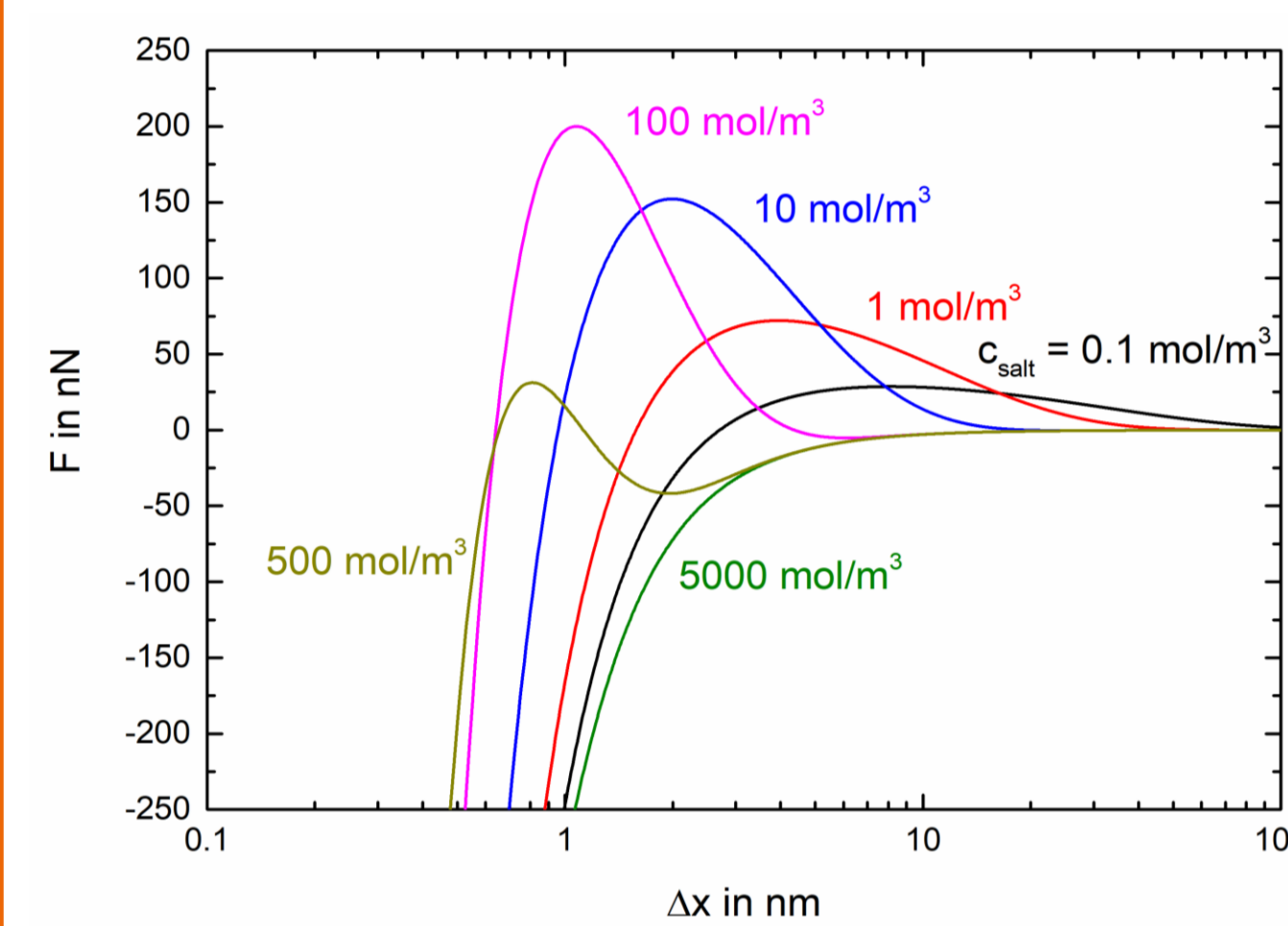


Figure 3. Typical evolution of the DLVO force with the distance between two drops [4]

- DLVO theory describes the force resulting from the repulsive ionic and the van-der-Waals forces acting between two approaching drops
- DLVO theory can be used to explain the salt influence on the coalescence [4]
- for the salt concentration, which induces a maximum force, the repulsive force between drops is large and hinders the coalescence [4]
- DLVO theory is introduced into the coalescence model

## Material and Method

- system paraffin oil + deionized water with salt is chosen in order to play easily with the viscosity
- different paraffin oil viscosity and salt concentration are tested
- ReDrop simulation will be compared to the settling experiments in order to validate the coalescence model

Table 1. Density and viscosity of a specific studied system

		25°C
saturated paraffin oil	density (kg/m <sup>3</sup> )	819.597
	viscosity (mPas)	8.48
saturated deionized water + 50 mmol/L of NaCl	density (kg/m <sup>3</sup> )	999.041
	viscosity (mPas)	1.030

- the two-phase system is stirred during 30 sec at 800 min<sup>-1</sup>
- experiments are conducted 3 times to validate reproducibility
- the settling time is reached when only half of the interface remains covered by a monolayer of droplets
- experiments are recorded on video in order to obtain the experimental data point
- SOPAT inline probe is used to measure the initial drop-size distribution

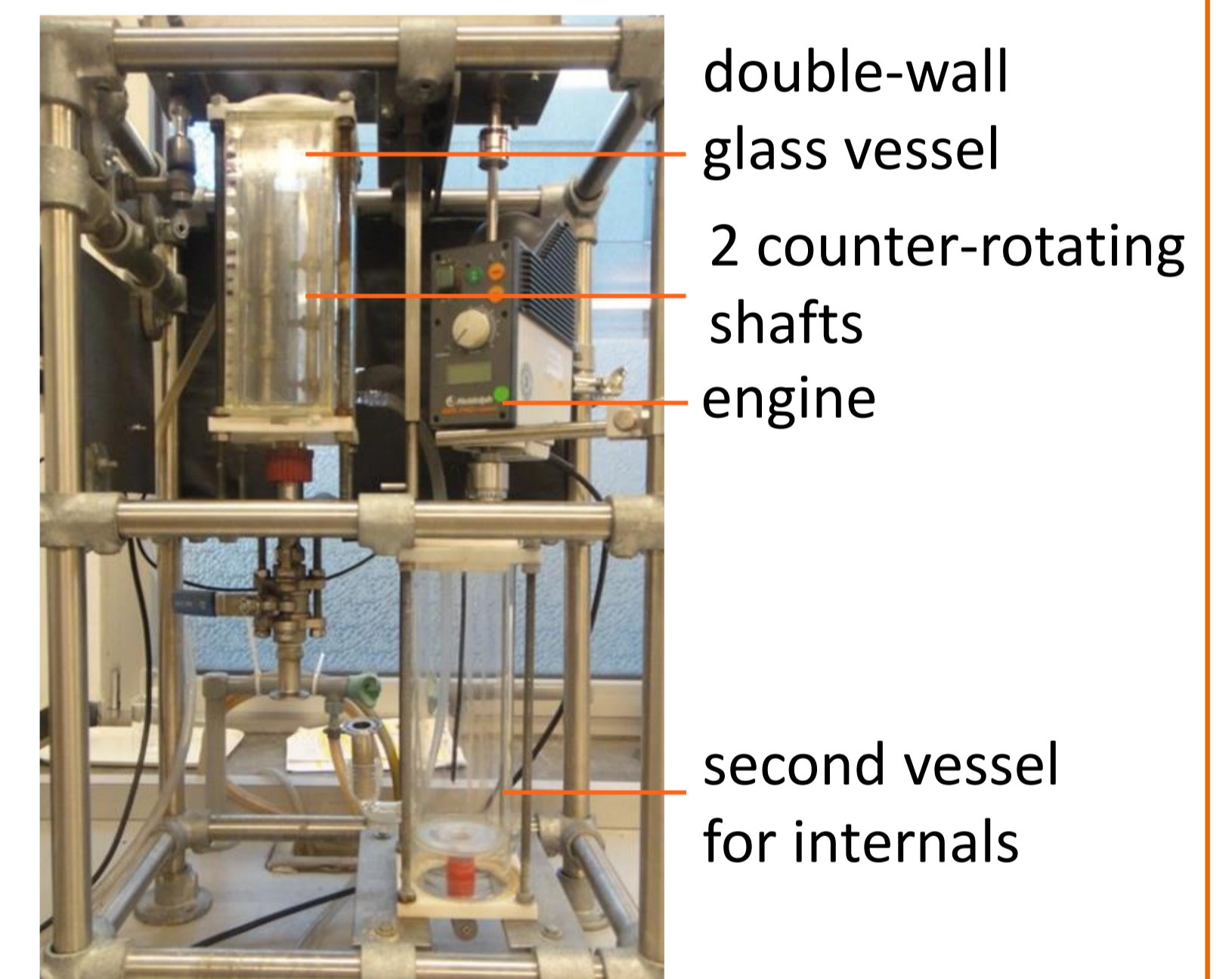


Figure 4. Henschke settling cell

## First results

### Collision rate

- the collision rate depends on the diameters of the drops,  $d_1$  and  $d_2$ , their height in the settling cell,  $h_1$  and  $h_2$ , on the relative velocity,  $v_{rel}$ , and on the area of the cell,  $A_{cell}$ :

$$r_{collision} = \frac{\pi(d_1+d_2)^2 v_{rel}}{A_{cell} |h_1-h_2|}$$

### Contact time

- equation of motion of two drops following their own curvature was solved to get a first impression of the contact time, the results are shown on figure 5
- further studies will combine this approach with further details of the relative motion, e.g. fluid dynamics, surface properties

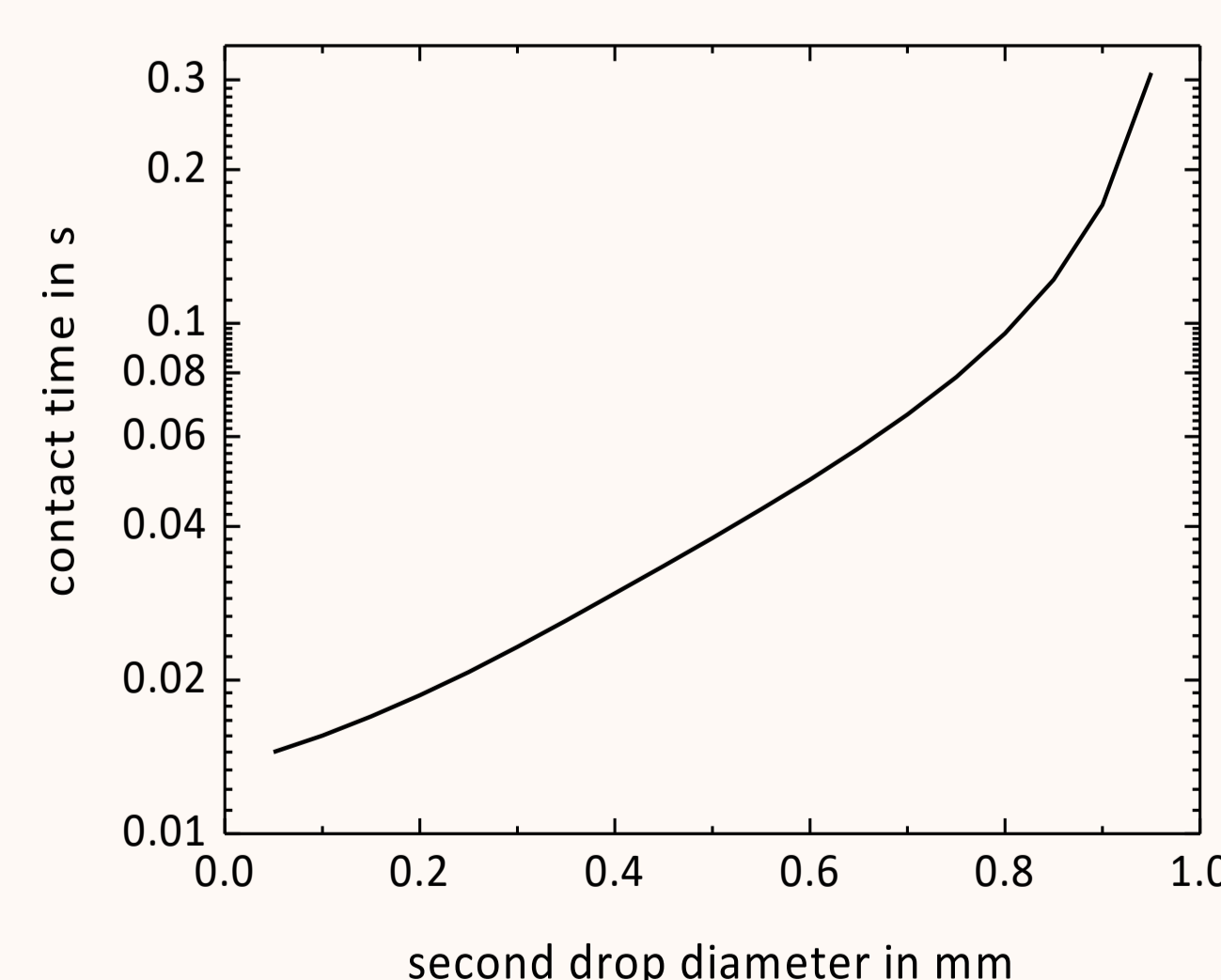


Figure 5. Contact time between a first drop of 1 mm and a second drop with varied diameter

## ReDrop simulation

- Coulaloglou & Tavlarides model [5] was first used to describe the coalescence time. DLVO theory has been introduced and will be tested.
- modeling of the coalescence curve will be implemented as a next step
- curved sedimentation curve and remaining drops are observed during the experiment and simulated with the ReDrop program

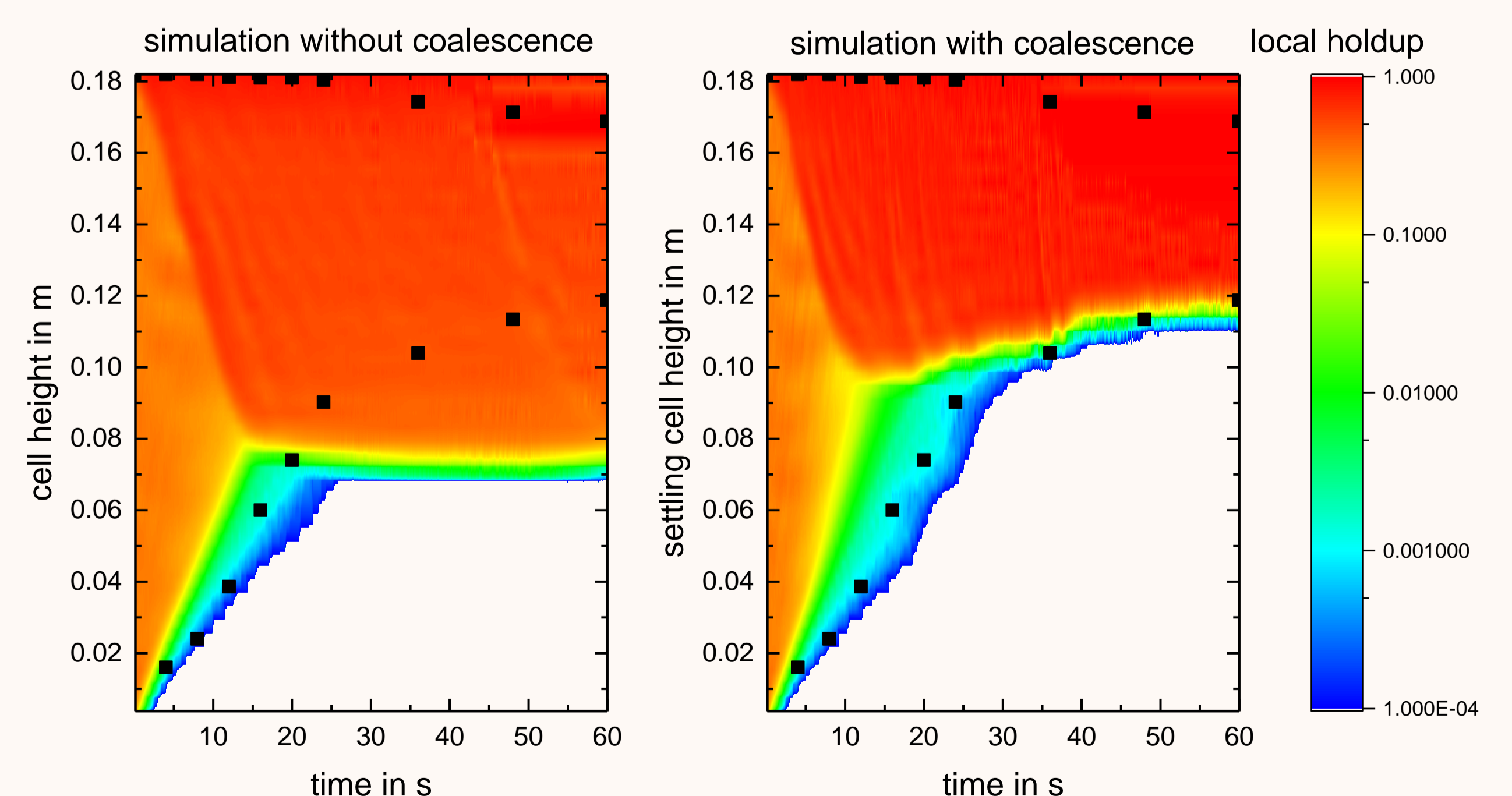


Figure 6. Simulation of settling experiment with the ReDrop tool.

## Conclusion

The simulation of settling experiments with the ReDrop program is in good agreement with observations. As next steps, further investigations will validate the DLVO theory in the coalescence model and will include the modeling of the coalescence curve in the simulation.

## References

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