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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.

## 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

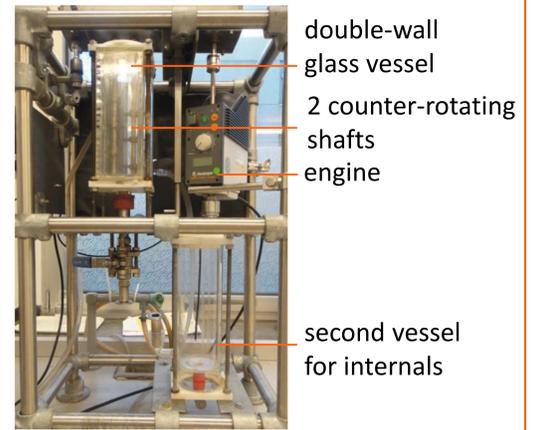


Figure 1. Henschke settling cell

## 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

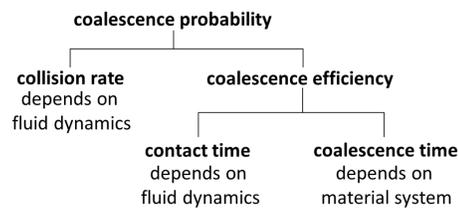


Figure 2. The coalescence model [3]

## 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,  $A_{cell}$  and on the correction factor,  $\gamma$ , which takes into account the reduction of the free volume:

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

## Coalescence time

- the coalescence time is evaluated by the balance between the fluid-dynamic force induced by the film drainage and the buoyancy force, which is the driving force of the coalescence phenomenon during the settling. The asymmetric dimple model of Henschke was applied [1].

## Coalescence efficiency

- the coalescence efficiency depends on the contact time, which can be, conceptually divided into time step,  $\Delta t$ .
- for each time step, a probability of non-coalescence can be defined as  $p_{non-coalescence, \Delta t}$ . For  $2\Delta t$ , the following has to hold:

$$p_{non-coalescence, 2\Delta t} = p_{non-coalescence, \Delta t}^2$$

- the probability of the entire process is,

$$p_{coalescence} = 1 - \exp\left(-\frac{t_{contact}}{t_{coalescence}}\right)$$

## Contact time

- equation of motion of two drops following their own curvature was solved to get a first impression of the contact time,  $t_{contact}$ , the results are shown on figure 3
- model found in the literature [6] fits to the simulation

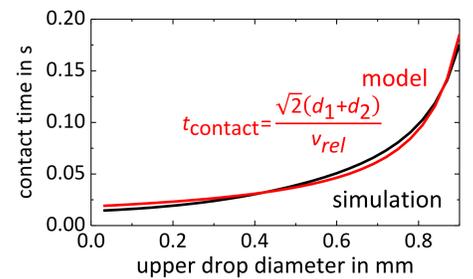


Figure 3. Contact time between a first drop of 1 mm and a second drop with varied diameter

## 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 in sedimentation and close-packed zone and with the major interface

- 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
- drop-drop and drop-interface coalescence is accounted for during the simulation
- deformation of the drops in the close-packed zone due to hydrostatic pressure modelled
- ability to record the drop-size and the local holdup at a specific time and height for further validation

## First results & Perspectives

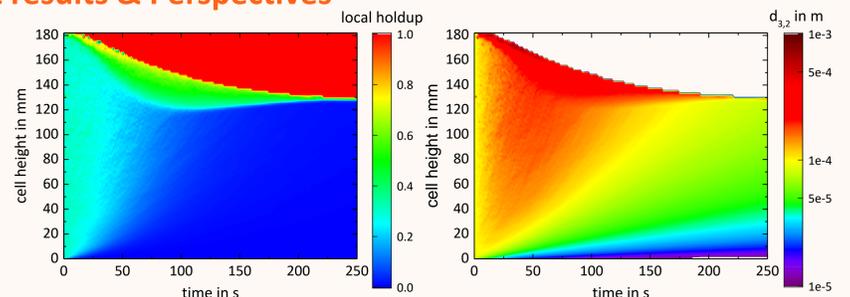


Figure 4. Redrop Simulation representing the evolution of the local holdup (left) and of the Sauter mean diameter (right)

- the ReDrop program can mimic system with curved sedimentation profile, as shown on the left side of Figure 4.
- the evolution of the Sauter-mean diameter shows small dispersed drops in the continuous phase at the end of the simulation. This effect is observed during experiment by a turbid continuous phase.
- as a first conclusion, the ReDrop simulation can mimic effects observed during settling experiment.
- as a next step, settling experiment will be compared to ReDrop simulation in order to validate the coalescence model

## References

- [1] M. Henschke, L.H. Schlieper, A. Pfennig, *Chem Eng. J.*, **85**, 369-378 (2002).
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- [6] J. Kamp, M. Kraume, *Chem. Eng. Sci.*, **156**, 162-177 (2016).

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