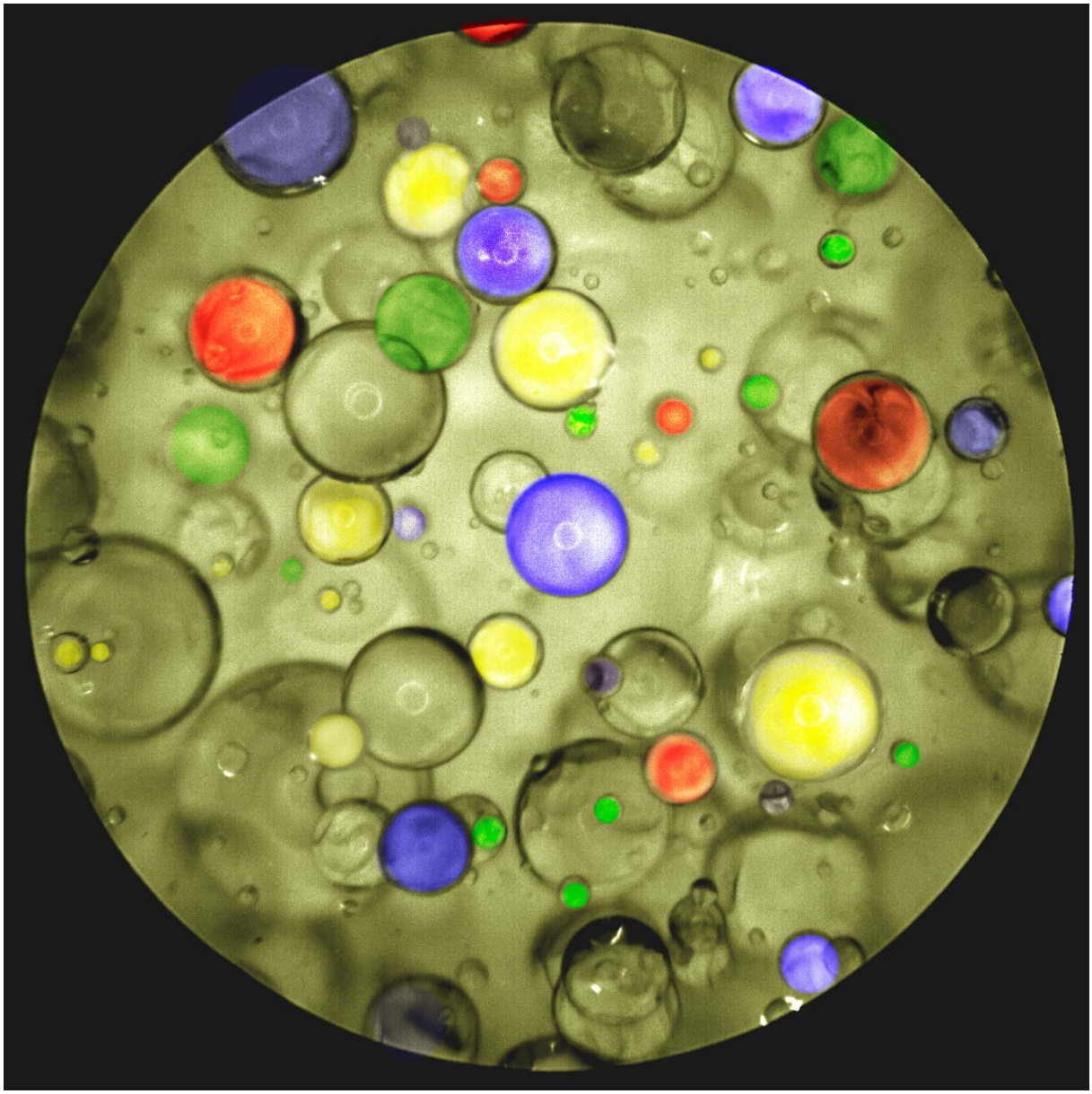
LIÈGE université

PEPs CHEMICAL ENGINEERING

Separation and Purification



2017

Content

title photo by:
David Leleu, Thierry Salmon,
showing a picture of a dispersion as seen by a SOPAT probe, https://sopat.de/en/

Dear Reader

As the year is coming to a close, on the one hand things are becoming a little hectic because they have to be completed by the end of the year. On the other hand, reflections on the year that passed come into mind. This year appeared quite filled with events and at the same time some larger steps become visible in projects and otherwise. In this brochure we will share some of these impressions.

During the year we had two visitors in our group. On the one hand Ms. Marjan Mohammadi Sarab Badieh visited from the Bu-Ali Sina University in Iran, where she is supervised in her almost completed Ph.D. studies by Professor Javad Saien. She made her first appearance in the annual report already last year and in this year's annual report can present her results on single-drop experiments with ionic liquids for sustainable extraction processes.

Our second guest was Mr. Khang Vu Dinh from the University of Industry in Ho Chi Minh City in Vietnam, where he is supervised by Professor Anh Le Hung. He has recently started with his Ph.D. project, which will be jointly supervised between Vietnam and ULiège, where here also Professor Angélique Léonard will be co-supervising. The project will be oriented in a similar direction as the PhosForYou Interreg project and work on establishing recovery processes for phosphorous from waste water or sewage sludge in a Vietnamese context. Thus quite some synergies can be expected between these projects.

A prominent event this year was the ISEC in Miyazaki, Japan. At the ISEC we were able to present a good overview over our recent research result, see Fig. 1. Of course being to Japan is also an experience in itself.

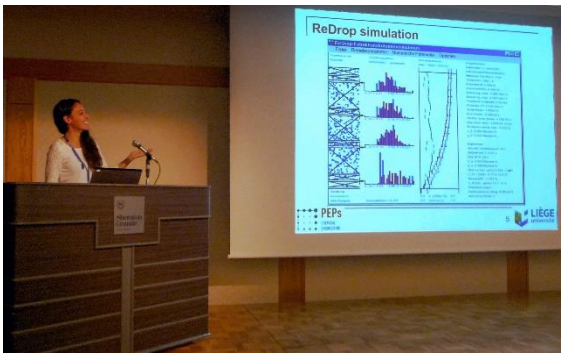


Fig. 1: Maria Chiara Quaresima reporting about her single-drop experiments at the ISEC in Miyazaki, Japan

Concerning research, our single-drop equipment is meanwhile in full operation and results are continually coming in. Thus, now the next challenges in solvent-extraction equipment design can be tackled. In coalescence modelling we believe that we made a big step forward based on a detailed analysis of the effects occurring during drop contact. This allows to propose a coalescence model, the structure of which is more consistent than previous approaches. And finally many side aspects positively developed, about which we also report in this brochure.

Enjoy reading!

Andreas Pfennig

Standardized Settling Cell to Characterize Liquid-Liquid Dispersion

David Leleu

Motivation

Continuous settlers are used in many processes for separating liquid-liquid dispersions. In an efficient process, this downstream operation must be sufficiently well designed. Since coalescence depends strongly on trace components, the dispersion needs to be characterized experimentally for each material system of interest, e.g. with respect to settling time. This can be realized in a standardized settling cells at lab scale. Different standardized settling cells have been developed which lead to different characterization procedures and results. It would thus be desirable to find an optimal standardized settling cell.

In the framework of the joint project “Energie und Ressourceneinsparung durch Innovative und CFD-basierte Auslegung von Flüssig-Flüssig-Schwerkraft-Abscheidern”, or ERICAA, funded by the Federal Ministry for Economic Affairs and Energy, the goal is to design one single standardized settling cell with optimal properties, which allows reliable evaluation of settling behavior and thus also an easier exchange of results between all project partners. One sub-goal of the project is to compare the different standardized equipment present at TU Kaiserslautern, TU Berlin, and at the University of Liège in order to build a new equipment which takes all positive aspects into account.

Experimental Setups

Two different settling cells were studied. The Henschke settling cell (Henschke et al., 2002, Schlieper et al., 2004), shown in Fig. 1, consists of a double-wall glass vessel with a capacity of 800 ml, with 2 shafts for stirring with 4 stirrers on each shaft. They are connected with a gearbox and are counter-rotating in order to allow quick decay of turbulences in the first seconds after switching off the stirrers without the need of baffles. The gearbox is driven by a stirrer motor. The double-wall of the vessel is connected to a thermostatic bath at e.g. 25 °C. The experiment is finished when only half of the interface remains covered by a monolayer of drops, leading to the so-called settling time. At the same time, a video recording of the cell during the experiment allows quantitative evaluation of sedimentation and coalescence curves, which are then used in the evaluation to obtain the required system parameters.

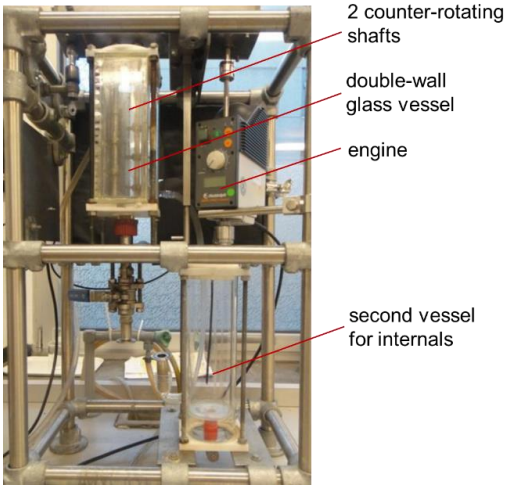


Fig. 1: Henschke’s stirred settling cell

The second settling cell is based on dispersing by shaking and has been designed at TU Berlin (Villwock et al., 2014), now also used at TU Kaiserslautern. The corresponding equipment built at the University of Liège is shown in Fig. 2. To control the reproducibility of the experiments, two bottles of 100 ml each are filled with the phases at identical phase ratio. These two bottles are mounted on an eccentric drive, which is connected to an electrical motor, which induces a vertical motion of the bottles. To create the dispersion, the bottles are shaken for 5 seconds. Settling experiments are recorded with a video camera as well. The frames are later numerically analyzed and their changes in grey level are used to evaluate the settling time.

Both cells have been built and dedicated experiments were performed and evaluated in order to point out the strengths and the weaknesses of each equipment for discriminating the optimal cell. Principal differences between

the cells are obvious. The effects which have been investigated in order to characterize the results of settling experiments are the four following parameters:

- the way of generating the dispersion,
- the influence of filling height,
- the possible air exchange with the environment, and
- the different evaluation methods.

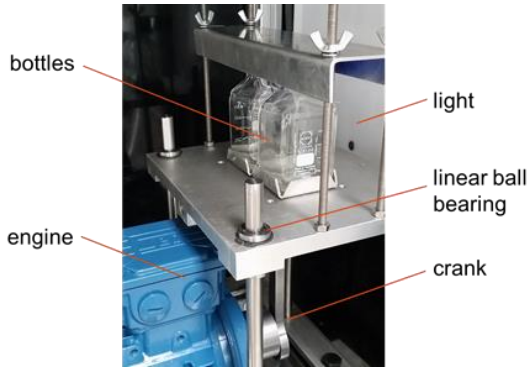


Fig. 2: Shaking cell

Results

First, regarding the influence of the characterization method, the visual criterion is preferentially used because it overcomes wall effects. When the interface at the center of the bottles is already cleared of drops, leading to the visual criterion being reached, there are still drops at the wall of the bottles, which strongly influence the numerical evaluation of the settling time from the videos, which only show the front view of the bottles. Thus the visual evaluation gives more reproducible results.

Secondly, The Henschke cell shows stability against the air exchange and the mixing intensity, characterized by the mixing time and the mixing speed as shown in Fig 3. The blue region corresponding to the stable region for the Henschke cell is much larger than the red one for the shaken cell. The last observed parameter, the filling height, does not seem to significantly influence the settling behavior for both cells.

As a general observation, the dispersion studied in the Henschke cell shows a settling behavior more independent of the operational conditions as compared to the shaking cell.

Based on this comparison study, the optimal settling cell was designed based on the Henschke cell. One major improvement consists in the use of the SOPAT probe for drop-size distribution measurement which is an important parameter influencing the settling. It should also be noted that the shafts are thicker compared to the former version of the cell in order to ensure more stable stirring.

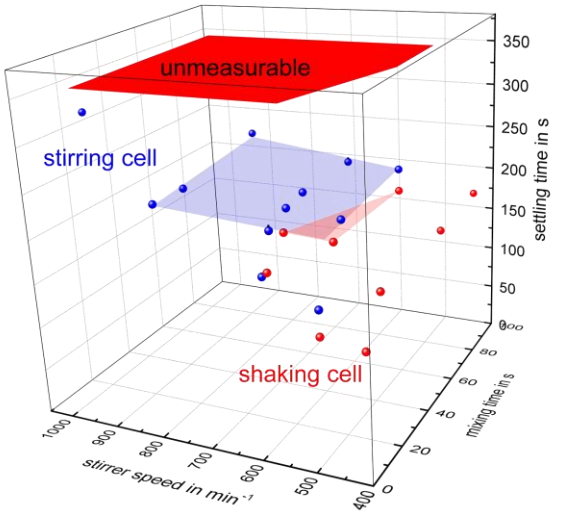


Fig. 3: Influence of the mixing time and the mixing speed

The settling time will be evaluated by the visual criterion as proposed by Henschke. The sedimentation and coalescence curves on the other hand will be automatically evaluated based on the video recording of the settling experiment.

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Coalescence in Highly Viscous Systems

David Leleu

Motivation

Molecules of common reactants for obtaining bio-based products contain a larger number of oxygen atoms as compared to fossil resources. Due to the resulting stronger intermolecular interactions, this will induce increased viscosities of the systems. At the same time, separation of liquid-liquid dispersions is a common task also in bio-based processes. Unfortunately, increased viscosity leads to comparably wide drop-size distributions, which pose additional difficulties in designing a technical settler, e.g. quantitatively predicting the remaining fraction of fine drops found at settler outlet as function of the operating conditions.

Trace components including ionic species considerably influence the settling behavior. The influence varies with the ion type and with their concentration making settling quite unpredictable. Thus, to quantify this influence for any technical systems, settling experiments are required, which can be conducted in a so-called settling cell. With detailed evaluation of such an experiment, the material system can be characterized by a coalescence parameter and by an initial Sauter mean drop diameter.

In order to simulate the separation of liquid-liquid dispersions and thus improve the design of equipment, a numerical tool has been developed, which is based on the ReDrop concept (Representative Drops). Sedimentation and coalescence are evaluated for a sufficiently large ensemble of representative individual drops at each time step. Both elementary processes are depicted by suitable models. Especially coalescence is a major challenge in these simulations.

Coalescence Model

As shown in Fig. 1, the frequency that two drops coalesce depends on the frequency with which they meet, defined by the so-called collision rate, and the efficiency with which they coalesce once they met. The coalescence efficiency in turn depends on the time, during which the drops stay in contact and the time they would need to coalesce. It turns out that solely the fluid dynamics of the regarded equipment determines the frequency with which drops meet and the time they stay in contact. The differences in equipment to which this model is applied characterize the fluid dynamics, which thus has to be characterized only once for a given type of equipment. The time the drops need to coalesce on the other hand only depends on the specific material system used.

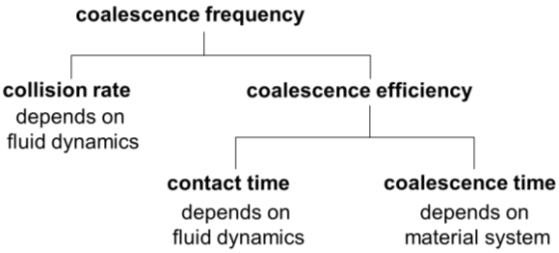

Fig. 1: The coalescence model (Kopriwa et al., 2016)

However, information concerning the collision energy is missing in this approach. Indeed, if the kinetic energy of the system is large, the drops will bounce and not coalesce. This has been demonstrated by Kamp et al. (2016), who finds that for high relative velocity the coalescence probability approaches zero, as shown in Fig. 2. Based on this assumption, additionally to the effects mentioned above, a probability of bouncing needs to be accounted for in the coalescence modeling.

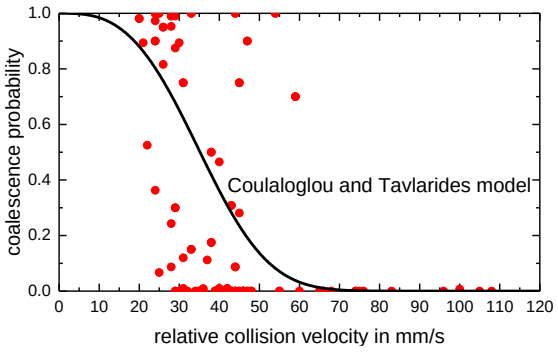

Fig. 2: Experimental data evaluated by Kamp et al. (2016) for a range of different drop sizes

A basis model was developed describing the phenomena, as depicted in Fig. 3: when two drops meet, they have a certain probability of bouncing, $p_{bouncing}$. If the drops stay in contact, they will follow their own curvature and during this time the coalescence process can take place as described above.

The overall equation describing the coalescence rate is thus given by:

$$r_{coalescence} = r_{collision} \left(1\text{-}p_{bouncing}\right) p_{coalescence}$$

The bouncing probability can be characterized utilizing a critical velocity, $v_{critical}$, as can be argued based on the data of Kamp, shown in Fig. 2:

$$p_{bouncing} = \begin{cases} 1 \text{ if } v_{rel} > v_{critical} \\ 0 \text{ if } v_{rel} \leq v_{critical} \end{cases}$$

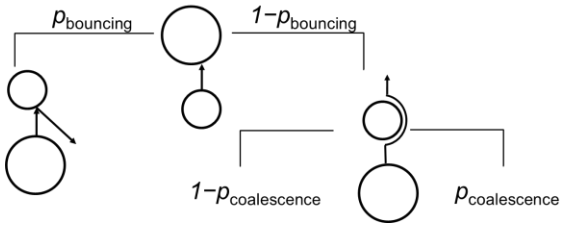

Fig. 3: General approach of the new coalescence model

When the drops stay in contact, coalescence can occur and is described by the coalescence efficiency. Conceptually, the overall contact time can be divided into time steps, Δt. For each of the time steps, the probability of non-coalescence can be generally characterized as $p_{non\text{-}coalescence,\Delta t}$. Then, for $2\Delta t$ the following has to hold:

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

Only an exponential function fulfills this boundary condition, which leads to define the overall coalescence efficiency as:

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

Even though this looks similar to previous coalescence models, the basic structure is distinctly different. The asymmetrical dimple model of Henschke is here used to evaluate the coalescence time.

Model Validation

The settling experiments are conducted in a settling cell as described in the corresponding contribution of this annual report. The SOPAT probe will be used to determine the initial drop-size distribution in situ, which is then used as starting condition in the ReDrop simulation. Different systems with increased viscosity to reach wide drop-size distributions and varied interfacial interactions introduced by small amounts of salt added will be tested and followed over time. The experimental results are used to validate the coalescence model.

The described coalescence model was implemented in the ReDrop tool. A simulation result is exemplarily shown in Fig. 4. The local holdup is represented by the color scale, the different lines follow a constant holdup along the simulation as well as the close-packed zone and the last drop in the simulation.

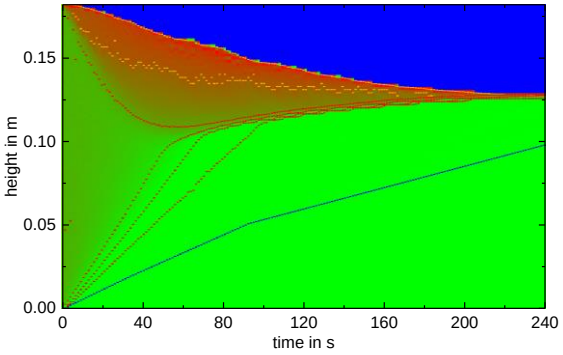

Fig. 4: ReDrop simulation using the newly developed coalescence model

References

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Performance Study of Ionic Liquid in Extraction Based on Single-Drop Experiments

Marjan Mohammadi Sarab Badieh, Maria Chiara Quaresima, Javad Saien

Motivation

Liquid-liquid extraction is mostly regarded as an alternative process for separation and purification, if vapor pressure of at least one of the components is low or the product is temperature sensitive. Traditional extraction methods typically apply organic solvents in contact with aqueous phases, but environmentally safe technologies may require alternative choices due to their toxicity, flammability, and volatile organic compounds (VOCs). To solve these problems, green solvents such as room temperature ionic liquids (RTILs or simply ILs) have been recommended recently as extractants in liquid-liquid extraction. Many ILs display outstanding properties such as negligible vapor pressure and tunable physiochemical properties. Therefore, they are known as “designer solvents” for particular applications. One of the well-known green ILs is 1-Hexyl-3-methylimidazolium hexafluorophosphate, abbreviated as $HMIMPF_6$ (see Fig. 1), which has a high capability as solvent in extraction processes. The extractive properties of this solvent can be demonstrated in the ternary system of water + acetone + $HMIMPF_6$. The liquid-liquid equilibrium (LLE) data of this ternary system, which are required for evaluating the performance of an extraction process, were reported to show a suitable partition coefficient (Saien et al., 2015).

In this work, the sedimentation velocity and mass transfer in the system water + acetone + $HMIMPF_6$ and the performance of $HMIMPF_6$ as solvent for the extraction process were investigated. Considering that ILs are relatively new solvents and thus their price for pilot-plant experiments compared to conventional extractants is high, design of the extraction system based on lab-scale experiments should be preferred, because this consumes less substances. To this end, single-drop measurements in a standardized equipment were applied, which contains two measuring cells for the lab-scale experiments: (1) the sedimentation cell for the measurement of drop velocity and (2) the mass-transfer cell for the determination of mass-transfer rate. Moreover, the experimental data have been evaluated using models developed for this purpose (Henschke and Pfennig, 1999). This method based on lab-scale experiments and modelling has been validated for a variety of system, mostly low viscous systems around 1 mPas or slightly viscous systems (Altunok et al., 2012). The influence of ILs high viscosity of 293 mPas is taken into account in the evaluation.

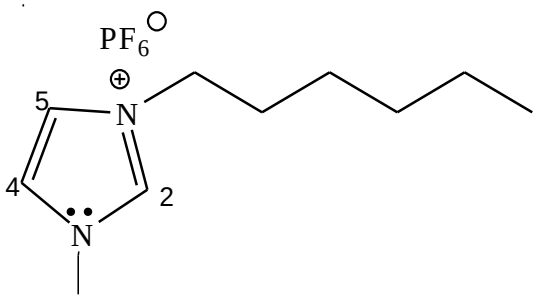

Fig. 1: The chemical structure of $HMIMPF_6$

Single-Drop Sedimentation Experiments

The experimental results of the single-drop sedimentation are shown in Fig. 2. The terminal velocity is shown as function of the drop diameter. The sedimentation velocity was fitted with the Henschke sedimentation model for the system water (c) + $HMIMPF_6$ (d).

The trend of the sedimentation velocity in Fig. 2 shows that it increases with increasing drop diameter until it reaches a plateau value at $v_\infty = 124$ mm/s around a drop diameter of $d = 3.5$ mm. The three parameters of the Henschke model (see e.g. Altunok et al., 2012) were then obtained by fitting to the experimental data: $d_{sw} = 2.53$ mm, $a_{sc} = 3.43$, and $a_{tr} = 2.2$. As a result, the Henschke model can be used to describe the experimental sedimentation velocities with good accuracy.

Single-Drop Mass-Transfer Experiments

The experiments on mass transfer in a single drop measuring cell were performed in the

available lab-scale equipment in order to obtain the instability parameter C_{IP}. Fig. 3 displays the dependence of the dimensionless driving concentration difference on contact time for a drop diameter of 2.43 mm. Fig. 3 also shows the comparison of the experimental results with the Newman model as extended by Henschke applied to the system water (c) + acetone + $HMIMPF_6$ (d). The dimensionless driving concentration difference decreases with increasing contact time, where comparing the results to previous experiments for systems with low viscosity mass-transfer is significantly slower. On the other hand, mass transfer turns out not to be as slow as expected due to the rather high viscosity of the system.

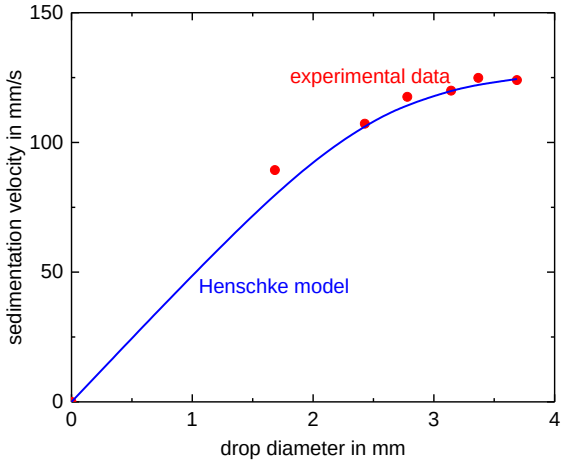

Fig. 2: Sedimentation behavior of $HMIMPF_6$ droplets in water

Fig. 3 shows that during the first seconds the experimental data systematically lie above the Henschke model. This may be due to the high viscosity of ionic liquid, so that it takes some seconds until the internal circulation inside the drop sets in and enhances mass transfer (Henschke, Pfennig, 1999).

To obtain an impression of the effect to be expected, the curve corresponding to a rigid sphere is included as dashed curve, which only considers molecular diffusion without accounting for the effect of internal circulation in the Newman model. The drop behavior will thus start out from the Newman curve and only after a transition over some seconds, during which the internal circulation develops, will reach the behavior described by the Henschke model. This transition behavior will be studied in future research in further detail. On the other hand, after internal circulation is established, the experimental results for the larger contact times are in good agreement with the Henschke model.

The experimental results successfully showed that this model can be also applied to the data obtained for the challenging system with ionic liquid. The corresponding material-specific model parameters were directly fitted and turned out to be for the effective diffusion coefficient D_{eff} =10^{-5} cm^2s^{-1} and for the mass-transfer parameter C_{IP} = 889.

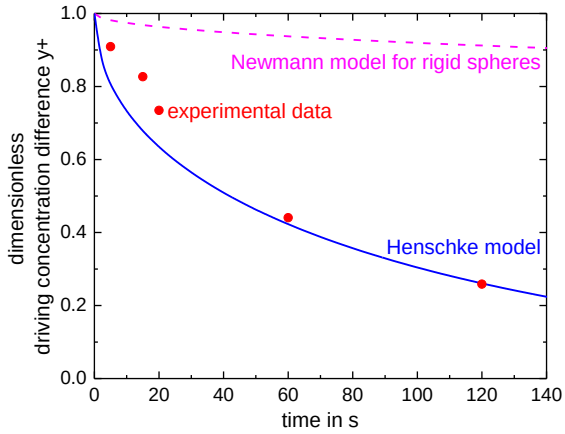

Fig. 3: Influence of contact time on mass-transfer in system of the water (c) + acetone (aq.) + $HMIMPF_6$ (d) and at drop diameter 2.43 mm.

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Extraction-Column Design for Viscous Systems

Maria Chiara Quaresima

Motivation

In the future, developing and implementing sustainable solutions for producing industrial materials will become a fundamental need. Today, the use of petroleum-based products and other non-renewable assets is depleting the world's natural resources. Thus, bio-based raw materials will in the future foreseeably replace fossil-based sources in chemical industry. This feedstock change will also lead to shifts in the molecular structure of reagents and products. The oxygen content in bio-based feedstock is higher as compared to fossil starting material. Processing a component, which contains significant fractions of oxygen on molecular level, will lead to intermediates and products rich in oxygen as well. Therefore, stronger molecular interactions due to polar interactions and hydrogen bonding will be present in such mixtures. This in turn will lead to lower vapor pressure and higher viscosity of the components. These changes in material properties need to be taken into account in process and equipment design. Since solvent extraction does not depend on vapor pressures, and in light of the future change in chemical feedstock, where more and more bulk chemicals will be produced from biomass, it will become increasingly attractive as a thermal unit operation.

Drop-Based Design of Extraction Columns

In the past, a design method for extraction columns has been developed, which is based on describing the behavior of individual drops in an extraction column (Altunok et al., 2006). The drop-models applied contain material-specific parameters that are fitted to results of experiments with individual drops in dedicated lab-scale experiments. These models are then combined in the simulation tool ReDrop (REpresentative DROPs). The idea of ReDrop is to follow a sufficiently large number of drops along their path in the column. This approach is capable of describing extraction-column behavior to better than 10% accuracy including the flooding point, being time and resources saving compared to pilot-plant experiments, which is the traditional way to design extraction columns.

In the past, already several studies have been performed, which allow first ideas on how systems with increased viscosity may behave. Especially Adinata (2011) performed a first orienting study on viscous systems. One of the results is that the parameter α_{sw} of the Henschke model for drop sedimentation (Henschke, 2003) describing the sharpness of the transition between rigid drops and drops with internal circulation has to be adjusted. These results are shown in Tab. 1. Originally, Henschke assumed that this parameter can be set to a value of 10 for all systems.

	system	α_{sw}
Henschke	d: *n*-butyl acetate c: water	10
Kalem et al.	d: isododecane + D2EHPA c: water + Zn + H2SO4	2
Adinata	d: toluene + paraffin c: water + PEG	5
this work	d: *n*-butyl acetate c: water + PEG	5.44

Tab. 1: Comparison of the sedimentation model parameters from different studies

As a consequence of this comparison, it is apparent that the viscosity influence on the sedimentation model needs to be investigated more systematically. Thus, the goal of this work is to extend the capabilities of ReDrop to account for systems with increased viscosity, which in turn will allow to solve the challenges described above resulting from the foreseeable shift towards bio-based feedstock.

As starting point, the sedimentation velocity of n-butyl acetate drops rising in a continuous phase of varied viscosity is investigated. As in the studies of Adinata, the viscosity of the aqueous phase is increased by adding PEG. The sedimentation velocity is determined in a single-drop cell shown in Fig. 1.

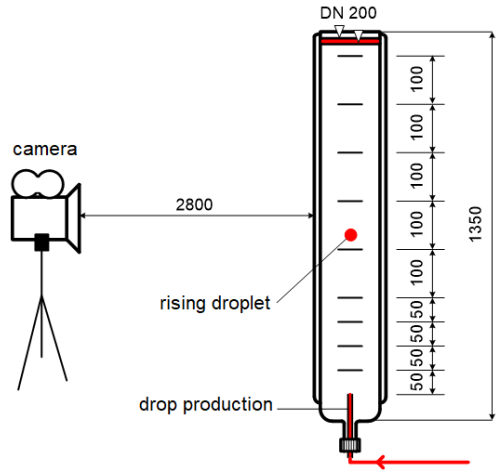

Fig. 1: Sedimentation cell for the measurement of single-drop terminal velocity

The cell consists of a cylindrical vessel, maintained at a temperature of 20°C. Inside this vessel a drop of known volume is produced with the help of a computer driven syringe, which can inject via a glass nozzle a defined volume of dispersed phase at a defined velocity. The glass nozzle is installed in the vessel and connected to the syringe by a PEEK hose of suitable diameter. By finding the right amount of dispersed phase to inject and the right velocity to correctly produce one single drop, individual drops with identical drop diameter can be generated. Each drop detaches from the glass nozzle tip and its path is recorded with a high-resolution video camera.

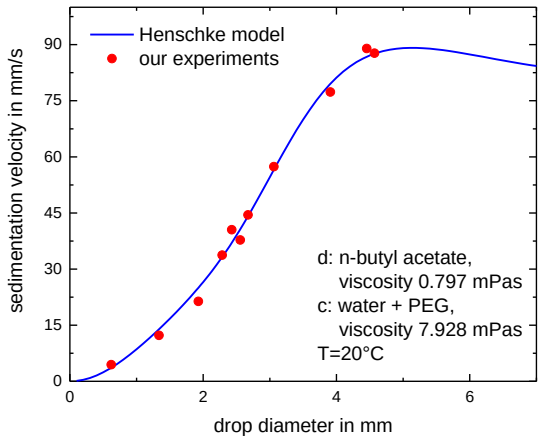

Fig. 2: Sedimentation velocity of n-butyl acetate drops rising in the aqueous phase as a function of drop diameter

Knowing the numbers of frames, and consequently the time, needed for the drop to rise in the continuous phase through a defined distance, sedimentation velocity can be easily determined. The Henschke model is then fitted to the experimental results in order to minimize the error between data and expected values. The results of a series of such experiments including the fit with the Henschke sedimentation model are shown in Fig. 2.

As expected, the increased viscosity of the continuous phase significantly slows down the droplets as compared to a low-viscosity continuous phase, where drop velocity easily reaches values well above 100 mm/s. As expected, also the model parameters are influenced by the viscosity variation. The corresponding first result is also included in Tab. 1.

Mass transfer is also expected to be slowed down by an increase in viscosities, which will be quantified in a next step of the project. The viscosity of the aqueous phase will be systematically varied by the addition of PEG and that of the organic phase by addition of paraffin oil. Then, finally, the new models will be implemented in ReDrop, which is then validated by corresponding column experiments. This will prepare ReDrop to be ready for the challenges induced by a more bio-based chemistry as described in the introduction.

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PhosForYou: Phosphorous Recovery from Wastewater and Sewage Sludge

Zaheer Shariff

Phosphorous and Wastewater

Phosphorous (P) is an essential element for life and has a limited availability in nature. Mineral P is mainly produced from phosphate rock, in the EU more than 90% of P used is imported to meet its requirements. Therefore, phosphate rock was classified by the European Commission as a critical raw material in 2014. A large proportion of P used as fertilizer in production of food as well as detergent and is finally ending up in the wastewater. If the phosphorus from wastewater is not removed, it leads to eutrophication in the receiving water bodies. Therefore, the waste-water treatment plants (wwtp) are required by law to eliminate P from their effluents. More than 90% of P is typically removed from wastewater by precipitation or by microbial assimilation and ends up in the sewage sludge. According to the national P budgets in Central Europe, the P content in wastewater can replace about 40 to 50% of P annually required for fertilizer production. In order to reduce EU's dependency on imports of P and to ensure sustainability, recycling of P from waste streams that otherwise would be lost to landfills has gained considerable attention in recent years.

The P4U Project

The PhosForYou (P4U) project funded for four years from 2016 to 2020 under the Interreg North-West Europe Program (see Fig. 1) is aiming at improved recovery of P from municipal wastewater, which could substitute about 26% of mineral P demand in North West Europe. The main goals of the P4U project are:

- building and testing P-recovery demonstrators at different wwtps
- demonstrate innovative P-recovery technologies
- develop new recycled P products for fertilizers
- working on a standard to assess recycled fertilizer quality including LCA of the technologies developed
- addressing social acceptance of recycled nutrient products.

Overall, six P-recovery demonstrators applying different technologies will be built by the partners and tested in real life conditions during the project. The P4U project is led by Emschergenossenschaft and Lippeverband (Germany) and has 12 partner organizations from 6 EU member states and Switzerland.

Fig. 1: Phos4You project theme

Work at ULiège

A new P-recovery technology (**Fehler! Verweisquelle konnte nicht gefunden werden.**) will be developed at ULiège aiming at recovering P from partially dried sludge followed by extraction of heavy metals to obtain a high quality P product that can be used for fertilizer production. Further, it is also the aim to explore, if the heavy metals extracted during the process may be recovered as valuable side-stream. An LCA study of the various processes developed by the P4U partners will also be carried out. The work at ULiège will be executed under the guidance of Angélique Leonard who specializes in LCA and sludge treatment and Andreas Pfennig who has expertise in separation processes especially solvent extraction. Laurent Fraikin will work on the processing of sludge before and after P recovery and conducting the LCA study, while I will work on the P recovery and refining processes.

Initially experiments will be conducted at lab scale for primary screening of the individual unit processes before building up the pilot plant. The method of cascaded option trees will be used

for designing and optimizing the process, which allows systematic bookkeeping of the various options available and keeping track of the feasibility test with respect to the critical criteria.

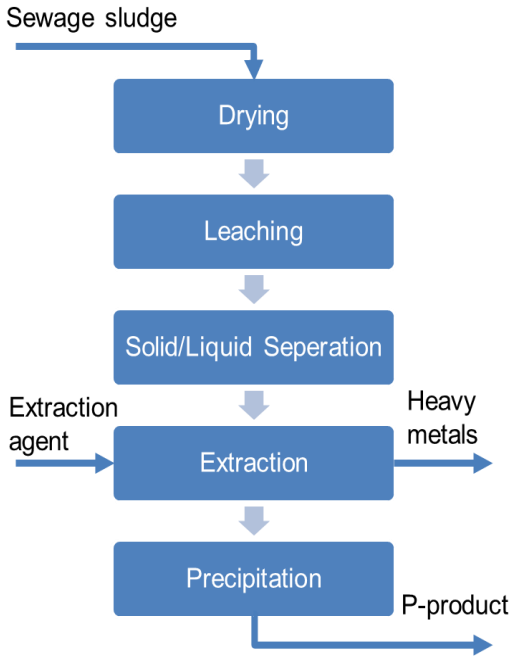

Fig. 2: Simplified process flowsheet of the P-recovery process to be developed

The ULiège process will be based on the PASCH process, which was developed at RWTH Aachen. In the original PASCH process, incinerated sludge ash is used as the input material for P recovery. The process that will be developed at ULiège aims at using partially to completely dried sludge as the input material so that the P-recovery may be carried out on-site without incineration. One of the main challenges in the recovery of P from sludge is the dissolution of biologically bound P, which is not required when working with incinerated sludge ash as all the biological matter is mineralized. Due to the use of components containing aluminum and iron for precipitation and removal of P during wastewater treatment, the leach liquor contains large quantities Al and Fe along with other heavy metals, which are present in smaller fractions. The solvent extraction used in PASCH process successfully removes most of the metals except for Aluminum. The ULiège process will apply the same scheme for heavy-metal removal by reactive extraction with co-extraction of Al, which will reduce the overall chemical consumption compared to the other P-recovery technologies from wet sludge.

After establishing and demonstrating the basic process on lab scale, a pilot plant will be built. The pilot plant will be designed to have a capacity of treating 5 to 10 kg of wet sludge per hour. As the plant is to be tested at various partner locations, it will be set up in mobile frames built from aluminum profiles so that it may be easily transported via truck. Within the framework of the P4U project, the pilot plant will be tested at wwtps in Belgium, Ireland, Scotland, and Germany.

The composition of wastewater and thus of sludge varies from one plant to another, so the operating conditions of the equipment will have to be optimized for individual situations using thermodynamic modelling and appropriate balances. A simulation model will be developed with the data gathered from literature, lab-scale, and pilot-plant experiments. The simulation model will help in accounting for the changes in boundary conditions and thus optimizing the efficiency of the equipment and technology for varying conditions. These variations include the boundary conditions of each specific wwtp but e.g. also changes of sludge composition during varying times of the year. The model will not only assist in carrying out simulations to optimize the process but will also provide the basic data required for detailed LCA and cost estimation. Based on the data obtained from the experiments on pilot-plant scale and the simulation model, finally a technical-scale equipment will be designed.

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On the Strong Effect of Faraway Molecules

Andreas Pfennig

Starting Point

In the context of molecular-dynamics simulations the question occurred, how the computer accuracy influences the results obtained. Computer accuracy is typically limited with double-precision variables to 16 significant digits. As a consequence, in any numerical operation random errors are introduced in the last significant digit. Thus, e.g. the position and velocity coordinates of the molecules experience random shifts on the level of this last significant digit at each time step.

Deterministic Chaos

To mimic the influence of limited computer accuracy, a single dedicated shift was introduced in a molecular-dynamics simulation of liquid water at 37°C with around 1000 molecules. This shift applied to exactly one molecule after thermal equilibration had been reached, which thus mimics a single numerical error. To be able to evaluate its influence, the shift of course has to be larger than computer accuracy. The magnitude of the shift was varied. The resulting molecular-dynamics simulation was then compared with a simulation without a shift. The deviation in position of the molecule, which had been shifted in one of the simulations, is shown in Fig. 1. It is apparent that with different initial shifts the development of the position deviation develops quite similarly. Only when the initial shift reaches computer accuracy, some variation is observed.

The development of the positional deviations between the simulation without and with the initial shift is essentially linear in the logarithmic plot over extended time periods. This behavior that a perturbation increases exponentially characterizes the system as being chaotic and displaying a so-called Lyapunov instability. Since the determining equations are exactly specified in principle, the behavior constitutes deterministic chaos. Only when the positional deviation reaches molecular scale, which occurs for the lines shown in Fig. 1 in the top right corner, the behavior is no longer exponential. Instead, diffusive behavior is observed, where the positional shift increases with the square-root in time as expected.

The exponential growth of the deviation has already been reported in the literature and is thus not unexpected. What may be a little surprising though is short time scale at which the deviation increases, which is also indicated in Fig. 1: The deviation increases by a factor of 10 every 0.23 ps. As a consequence, if a certain accuracy of a molecular-dynamics simulation shall be achieved, for every 0.23 ps simulated time farther into the future, the starting positions have to be specified by one more significant digit. Of course, actually also the computations would need to be performed with that quickly increasing accuracy.

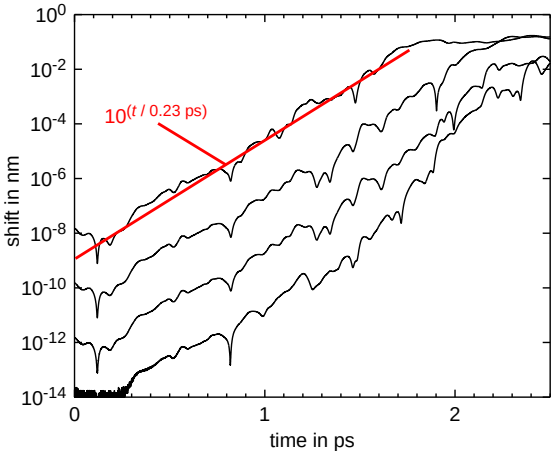

Fig. 1: Deviation in position of a molecule induced by a small initial shift in a molecular-dynamics simulation

Since the accuracy of typical computers is limited, e.g. to 16 significant digits, the numerical errors will dominate the molecular behavior after less than 4 ps. After that time, the numerical errors will have reached molecular scale and after that continue to grow with the speed of diffusion. As they reach molecular scale, the molecular motion is developing in essentially random direction as shown in Fig. 2, where small but different starting shifts have been introduced for each trajectory. Thus any real molecular-dynamics simulation will actually have to a significant degree the nature of a

Monte-Carlo simulation. Molecular dynamics thus very fundamentally does not allow to describe real molecular trajectories.

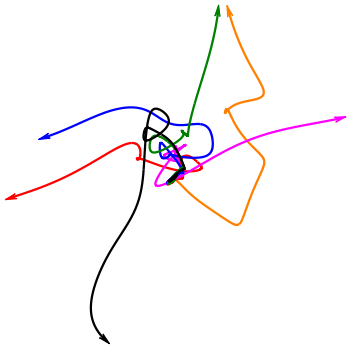

Fig. 2: Molecules quickly move in random directions, if small but different shifts are applied at start

As a consequence, the accuracy of prediction of individual molecular behavior with any realistically manageable effort even over intermediate times will remain limited. This is the usual way, in which deterministic chaos is characterized.

Influence of distant molecules

The question arises, if the results do also imply something on reality itself – and not just our disability to predict its behavior. To gain some insight, it has to be realized that any particle at a distance from the regarded system will interact with the system with an interaction force. To avoid complications, here only gravitation is regarded, which acts also over large distances. The farther away the influencing molecule is located, the smaller its influence on the regarded system will be. Nevertheless, the interaction force will lead to an initial shift in the position of all particles of the regarded system, which will increase by a factor of 10 in just 0.23 ps for the water system investigated.

To evaluate the influence of distant molecules on any target molecule in the regarded system, the question can be answered, how long it takes until the influence of a distant molecule reaches molecular dimensions. Such a shift would e.g. correspond to a bifurcation, where a target molecule 'decides', if it passes right or left of a neighboring molecule in a diffusive move. Since the interactions by gravitation to a first approximation can be regarded pairwise additive, the force as well as a starting shift induced for a target molecule corresponds to that contribution found in the concert of all interactions experienced as linear superposition by the target molecule.

The resulting time until an initial shift induced by a distant molecule in a target molecule reaches molecular dimensions is depicted in Fig. 3. It is apparent that even for very distant influencing molecules the time until a target molecule reacts is extremely small, namely at most 33 ps, even if the influencing particle is located at the end of the observable universe. This evaluation already accounts for the effect that the forces originating from a distant molecule acting on a target molecule and its neighbors are quite similar and only the difference may be accounted for, which is indicated as 'delta influence' in Fig. 3. Of course this short interaction time only arises after the interaction has reached the target molecule. Thus the target molecule interacts with a water molecule in Andromeda galaxy, which is roughly 2.5 million light years away, as it behaved 2.5 million years ago.

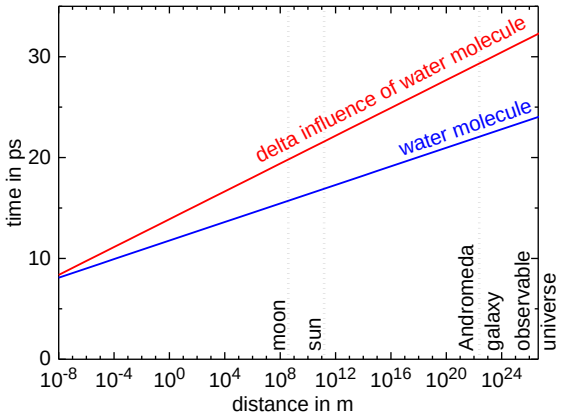

Fig. 3: Reaction time of a target molecule induced by a distant molecule

This effect does not only relate to our ability to describe the behavior of the system but to the interaction as it occurs in reality. To mention just some consequences: All particles in the universe are linked via a network of mutual interactions, which holistically determines their individual future behavior. As a consequence, the concept of causality cannot be applied to molecular motion. Also isolated systems, often applied in thermodynamics, cannot be practically realized.

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Videos on YouTube: Expert Course on Extraction

Andreas Pfennig

Background

In the last years' annual report the YouTube video series for the lecture on thermal separation processes has already been introduced. This video series meanwhile consists of 34 videos varying in length between roughly 15 and 50 minutes. The content is presented together with corresponding manuscripts in a structured way on the following website: http://www.chemeng.uliege.be/PUO1, where the English version of that page has to be selected.

In the meantime it turned out that even in industry cooperations these lectures are helpful. In one case the video on general assumptions and conditions of applying the McCabe-Thiele method was recommended. If the graphical step-construction or correspondingly the short-cut equations shall be applied, the flowrates have to be chosen such that they are constant throughout the counter-current process. If e.g. in solvent extraction a transfer component with a high starting concentration is extracted, the overall flowrates may strongly change along the extraction column. In that case the assumption of constant flowrate is often better matched for the carrier flowrates, i.e. those of the primary solvent and extractant. This directly implies that loads (mass or amount of substance ratios) are to be used as concentration measure, i.e. the mass or amount of substance ratio between transfer component and carrier component of the respective stream. This has to be used consistently, i.e. the equilibrium has to be expressed in these concentrations as well. When the corresponding short-cut equations are to be used, of course also the partition coefficient has to be evaluated for these concentrations. If instead the overall flowrates and correspondingly mass or mole fraction are used, the resulting number of theoretical stages may turn out to be quite wrong.

Meanwhile some of the lectures have been synchronized in Brazilian Portuguese. Also the number of followers is steadily increasing. We are also happy that the link to the videos is even mentioned in the news on the EFCE website – of course without us having asked for it: http://efce.info/Fluid+Separations.html. And of course we agreed to use the links.

Further videos for this series are continually recorded, which is an ongoing project. It should be mentioned here explicitly that the videos are published with a creative commons license by-nc-sa, i.e. they may be used and even modified, but the authors have to be mentioned as indicated in the videos (by – attribution), this has to be non-commercial (nc) and if published, the new videos have to be published under identical boundary conditions (sa – share alike). Thus anybody can use the videos under these creative-commons terms. Linking to these videos and the website including the manuscripts is of course welcome.

The Idea

At the same time it has been realized that we are continually developing new knowledge by our research, which is 'only' presented in journal papers and on conferences. Journal papers usually treat the issues quite briefly and the basics are hardly completely described. The presentations on conferences are prepared with significant effort, i.e. nice slides exist for all of our research topics. But since the presentations are only experienced by the audience present, this is apparently fleeting effort. Finally, also for industry workshops on our research topics, completely worked out presentations with significant detail even including some derivations are available in our group.

Thus the idea arose to present large portions of this collected detailed knowledge in a didactically optimal way and make this publicly available. In some cases this requires that new slides are prepared for content, which is worked out in Ph.D. or even student theses. Also rather old diagrams, slides, and presentations have to be searched, because it occurs that much has already been worked out in principle but has been lost over the years in the depth of some hard drives. These diagrams possibly need some modern restructuring, but can often be used quite directly. The corresponding manuscript chapters of course have to be written as well.

Realization

Starting out from material collected for expert workshops, first videos have meanwhile been recorded for the advanced topics on solvent extraction. An example taken from a video on the electrostatics of interfaces is shown in Fig. 1. These videos and the corresponding material are again collected on a website in a structured way:
www.chemeng.uliege.be/extraction.

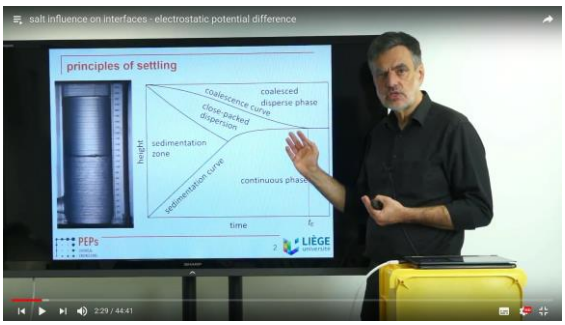

Fig. 1: Screenshot from the video on salt effects in solvent extraction

Currently, the following topics have been worked out and are in preparation (in shades of grey):

- cascaded option tree and optimal solvent selection
- salt influence on interfaces
  - electrostatic potential difference
  - interaction of several salts
  - quantifying the potential difference
  - effects relevant for solvent extraction
- crud
- drop-based extractor design
  - drop sedimentation
  - mass transfer without internals
  - internals influence on mass transfer
  - drop coalescence
  - drop splitting
  - ReDrop simulations
  - application to challenging systems

The topics thus essentially cover all areas of our major research expertise. It is also apparent that certain topics are still missing, for which the structure and videos will be worked out in the future. This includes some topics, which are already covered in our lectures, e.g. on reactive extraction and mass-transfer induced instabilities.

One major goal of the video series is to present the content not just as in scientific journals or on conferences, where the fundamentals are usually only briefly mentioned. Instead the goal is to work out the topics in a didactically optimal way. This includes e.g. derivation of the major equations, which allows to apply the concepts also to different areas. Of course the video series on our collected extraction knowledge also cites the basic lectures e.g. on the McCabe Thiele diagram.

The lecture material will also be used in an advanced lecture at the University of Liège, which has been presented for the first time this academic year: “Process Intensification and Hybrid Processes”, where the drop-based design methods are one way of reducing design risks and thus the safety factor for equipment design, which in turn leads to a reduction in equipment size and holdup, i.e. an intensified process.

Invitation to Others

Since in a university environment e.g. large-scale equipment as well as a variety of practical issues like trouble-shooting cannot be properly addressed, other experts in the field are invited to contribute, e.g. with videos, which can be recorded in our studio. Also it turns out that it is significant effort to obtain photos and especially video clips of large-scale equipment and test facilities. While all companies asked so far were quite supportive, nevertheless for each individual photo, diagram, video, etc. the copyright issues need to be addressed. Here also support from companies with respect to real-world photos, graphs, and videos is very welcome. Of course appropriate credits will be given. Since also problematic cases with e.g. corroded examples would be welcome, confidential treatment of the source can be ensured as well.

It is hoped that the material and videos may in the future serve as a first step to acquaint oneself with solvent and reactive extraction also in an industrial environment. Even, if all the details e.g. on drop-based design may not be directly applicable, the videos tell a story which may serve as a background to understand some of the challenges experienced in design and operation of extraction equipment.

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Easter Activity of the Chem. Eng. Department

Maria Chiara Quaresima

On a sunny afternoon on April 4, 2017, the staff of the Department of Chemical Engineering ran into a stage race that took place in the midst of the Sart-Tilman campus. This departmental activity was organized with the aim of getting everybody involved and thus developing the team spirit among all the scientific, technical, and administrative staff.

Fig. 1: Team 5 at the race starting point, the *"Taureau"* by Francis André, 1984

Fig. 2: Team 1 with the artwork *"Sieste sur les hauteurs de Liège"*, by Patrick Corillon, 1996

Five teams were formed and the participants challenged in a race, the purpose of which was to reach several works of art within the university area, composing the so-called open-air museum. That the required works have indeed been reached had to be documented by photos, respecting some rules specified by the organization committee. In each photo, a given number of people of the team had to be present and every artwork had to be reached in the shortest possible time.

Fig. 3: Team 5 at the artwork *"Imago"*, by Emile Desmedt

Fig. 4: Team 5 at the *"Sculpture du Plan K "*by Félix Roulin, 1975

Beside the competition, a good atmosphere was created, thanks to the collaboration within the teams. It was a funny and relaxing occasion to know more about the people we work with every day. The prizes, consisting of candies and snacks, were awarded to the fastest team and that with the most original photo. Team 4 won for the most original picture but also for the fastest race together with team 3, in which one of our group members participated. A small victory that will motivate us to do better next year!

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SFGP Congress 2017

Maria Chiara Quaresima

The SFGP

The SFGP (Société Française de Génie des Procédés) brings together professionals in the field of process engineering in France: researchers, industrials, and equipment manufacturers coming from all relevant industrial sectors of activity. It has about 500 members. In order to promote the exchange of knowledge between the different actors, the SFGP has structured itself into 17 thematic groups and each of them organizes scientific meetings, debates, or symposiums by inviting people who have expressed interest in the theme. The SFGP organizes its annual congress to promote interconnection between all this expertise.

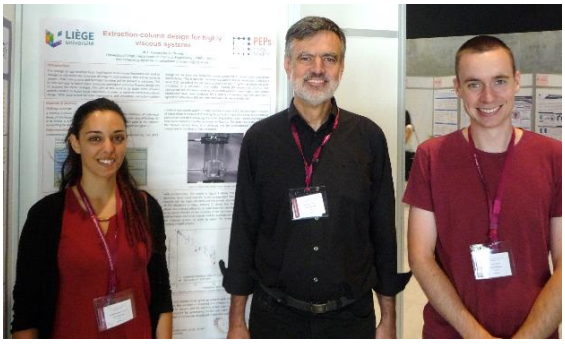

Fig. 1: Our team at the SFGP Congress.

SFGP 2017 in Nancy

From the 11th to the 13th of July, 2017, the 16th edition of the SFGP Congress took place in the city of Nancy. Nancy is an agglomeration with nearly 300 000 inhabitants, located in Lorraine (France), with a dynamic spirit aimed at innovation and creation, where knowledge and industries have always been linked. Nancy has some tourist attractions undeniable related to the Art Nouveau (School of Nancy) and at the Stanislas Square (see picture above), listed as a UNESCO World Heritage Site. In this years' SFGP annual conference 600 participants were present, coming from a dozen of different countries. During three days, 243 oral sessions and almost as many posters were presented. Five major themes were proposed as main topics of the congress:

- process engineering for the energy transition
- products engineering: from the molecule to the material properties
- process engineering as an answer to the 21st century environmental challenges
- process engineering for innovation in bio-productions
- focus on some cross-cutting theme.

Our team participated with a poster communication by David Leleu on standardized settling cell design for coalescence investigation in liquid-liquid dispersions and a poster by Maria Chiara Quaresima on single-drop experiments for extraction column design for highly viscous systems. Andreas Pfennig held an oral presentation on process design based on cascaded option trees. During the conference, the focus was placed on future process engineering and innovation. Many specific applications at an industrial and academic level were presented to face the big challenges of the future as indicated in the major themes. You can find more details on the conference website: www.sfgp2017-nancy.com.

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In Miyazaki, Japan: The 21st International Solvent Extraction Conference

David Leleu

After the last ISEC conference organized in 2014 in Germany, this year the International Solvent Extraction Conference took place in Miyazaki, Japan. The conference was organized in a conference center with associated hotel located directly near the ocean. More than 300 researchers, expert in extraction, participated in this 4-days conference in November 2017. Among more than 20 participating countries, the German community was well represented by the Universities of Aachen, Berlin, Kaiserslautern, and Dresden to mention just a few.

The City of Miyazaki is located in the South of the country at 900 km air-line distance from Tokyo. The city is famous for the golf courses and for their rock formation along the coast (see Fig. 1), which we had the chance to visit during an organized excursion.

Fig. 1: Rock formation at the coast

Our team was represented by Andreas Pfennig, Maria Chiara Quaresima and myself. We contributed three posters related to the design of extraction columns and to coalescence modeling. Three subjects were also delivered in oral presentations, one by each member of the group. Andreas took the audience behind the scenes of his YouTube videos on solvent extraction, Maria Chiara talked about her single-drop experiments used to design solvent extraction for highly viscous system and I presented the comparison between two settling cells used to characterize liquid-liquid dispersions (see the corresponding contribution to this report).

The subjects presented during the conference covered e.g. rather general topics mostly from the area of metal recycling, specific topics on dedicated processes, as well as fundamentals on developing understanding for the detailed phenomena taking place during extraction processes.

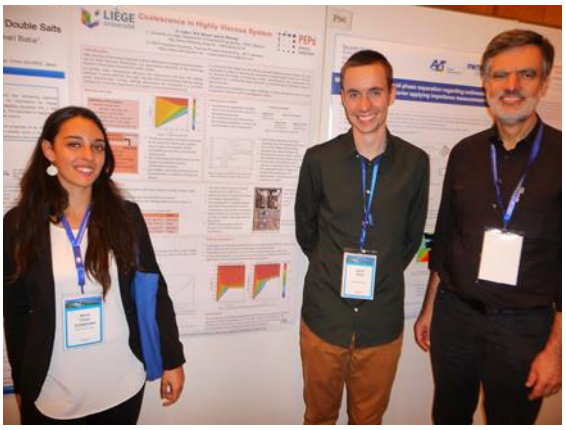

Fig. 2: Team present at the ISEC

Some companies were also present and exhibited their equipment ranging from measurement techniques as the SOPAT probe, used to measure drop-size distributions, to extraction columns. Two companies e.g. proposed extraction columns working at high holdup well above 50% in order to increase the separation performance, while usually lower holdup around 20% is desired for extraction columns.

During the last night on the occasion of the conference dinner, we enjoyed some delicious local dishes while listening to traditional Japanese music.

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Visit of the Recycling Center of BAV

David Leleu

Fig. 1: Panorama view from the top the landfill hill

In July of this year, Andreas and I visited the recycling center :metabolon of the Bergischer Abfallwirtschaftsverband, BAV. The goal of the meeting was to organize my secondment in the context of the Phoenix project, aiming at efficient utilization of bio-based resources, funded by EU in the context of the Horizon 2020 program.

Located 40 km east of Cologne, BAV is a recycling center where innovation and public awareness of waste management were developed over the years. It is built besides a waste dumpsite, which is now sealed. The education center :metabolon organizes awareness campaigns for young people. School classrooms and an exhibition hall are present on site. Several activity modules are located in different places of the center.

In the middle of the site a hill made of waste landfill accumulated over the years was equipped with a large children playground and bears a beautiful panorama view as shown in Fig. 1. Besides, scientific research projects have been developed, e.g. establishing a pyrolysis process in order to produce electricity. The raw material stems directly from the recycling center, which is shown in Fig. 2. The BAV also accommodates an on-site waste-water treatment plant to clean up the rainwater after becoming polluted because it came into contact with the contaminated soils.

My secondment will be focusing on the improvement of their separation process involving liquid-liquid dispersion. The settling behavior will be characterized in the standardized settling cell in order to optimize the system and to reliably design the equipment to be used on site.

This will be an opportunity for me to work in a different cultural and scientific environment and to share our both expertise. This secondment will also provide me with a different point of view on the research topic, because it allows to directly access real-world dispersions to be separated. In addition, the exchange program will give the opportunity for us to establish links, which can be the basis for future collaborations. The secondment will start in January 2018 and last for 6 months.

Fig 2: Biomass for the pyrolysis process

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New Website, E-Mail Addresses, University Logo

Andreas Pfennig

On the occasion of this year's 200th anniversary of the University of Liège the corporate design was modernized. The many colors in the new logo, shown in Fig. 1, represent the multi-cultural and multi-facetted structure and services of the university. The logo has the shape of a coat of arms on the one hand but simultaneously depicts an open book, which hints towards the openness for the future and to learning. This change in outer appearance shall be a first step in also renovating internal structures, which will of course take its time.

Fig. 1: The new university logo

At the same time the abbreviation of the university was changed. Formerly the cryptic ULg had been used throughout, which is now replaced by ULiège, which also conforms more to international standards in university acronyms. This is of course also reflected in the new e-mail addresses, which now have the ending '@uliege.be'. The old e-mail addresses will on the other hand remain working for an extended period of time.

Thirdly, also the university website has been newly designed, where the address now also builds on the new acronym: www.uliege.be. The look of the new website is modernized and it is clearly better structured, e.g. being oriented with respect to possible classes of visitors of the website. Some new animations realized e.g. on the main homepage appear to be some overshoot though, but it is expected that this will rectify over time.

The department has already been involved in the reworking of its website since quite the beginning of the redesign of the university website. After several new arrivals of scientific staff with new research areas, the department website called for a new structure as well. Since our request for designing a new website coincided with the decision of the university to restructure the entire university website, we acted as guinea pig for the newly developed structure. This involved various interactions with the computer center, the SEGI (Le Service Général d'Informatique), which was responsible for the realization, and a steering committee directly associated with the rectorate, which took care that the structures stayed consistent with what was originally intended. Internally the structure of our new department website has been worked out by a small team. This new website was also launched earlier this year. Its new address is – of course consistent with the changes mentioned above: www.chemeng.uliege.be, see Fig. 2.

On this website the three subgroups of the department are reflected, which present their individual expertise and research topics. For example the PEPs group (Products, Environment, and Processes), to which our working group belongs, presents its major research topics at www.chemeng.uliege.be/peps-topics. This new structure helps to keep the website content up-to-date so that you as visitor can always explore our current activities.

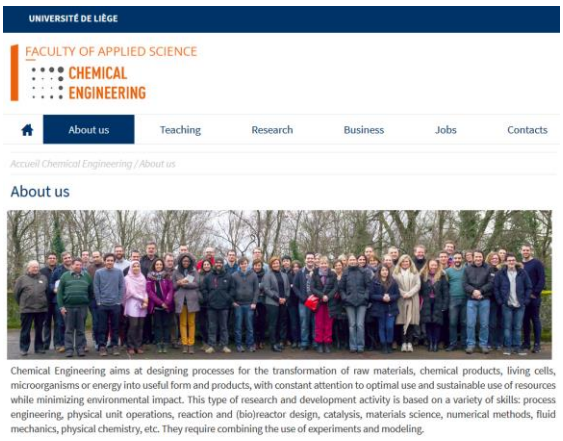

Fig. 2: The new Department website

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EFCE WP Meeting Fluid Separations

This year on May 11, the annual meeting of the EFCE Working Party Fluid Separations was organized in Liège with funding and support of Solvay. The venue of the technical meeting was the Opera Complex in the center of the city. The program was quite diverse and especially focused on new ideas and developments. Together with some of the contributions, it is available online on the EFCE WP website.

Fig. 1: Dr. Magdalena Bendová from the Institute of Chemical Process Fundamentals of the Czech Academy of Sciences presenting on Mathematical gnostics

On the second day, an excursion was organized to vito, a Belgian research organization, which is active "in the areas of cleantech and sustainable development, elaborating solutions for the large societal challenges of today." This applies among others to the areas of energy, materials, land use, and health. Especially impressive were the pilot-plant installations in which they performed the tests for the newly developed processes.

Fig. 2: At the excursion to vito

Teaching at GUtech, Oman

As in previous years also in 2017 a block course on Thermal Separation Processes was held at GUtech, Oman. It was organized during the last two weeks of May. Here apparently synergies evolve, because as a support to this block lecture, the YouTube videos can be used. Nevertheless, it is always a challenge to transfer the knowledge as a so-called fly-in, where both sides have to acquaint with respect to teaching and learning style within just some days. It is encouraging to realize that generally the motivation is quite high and some students are performing excellent.

Fig. 1: The students of this years' class

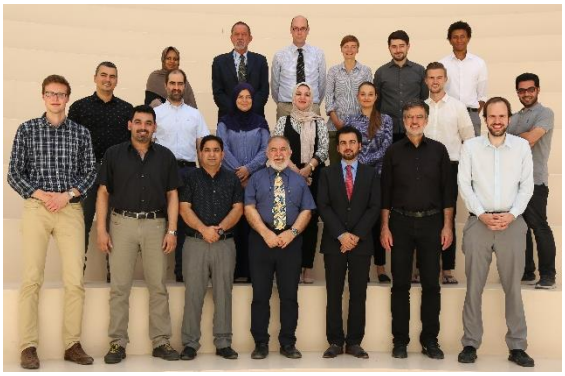

Fig. 2: The Engineering Department at GUtech with the rector, Prof. Michael Modigell

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The Schnapps Project 2017

Andreas Pfennig

Meanwhile the schnapps project has been established at ULiège. The formal procedures for obtaining the permissions have been worked out with the officials from the city of Liège and the university. Since we have the status of a licensed distillery, this is a little bit of effort. As long as we work properly, our case is luckily treated with a certain Belgian flexibility.

This year only five students had chosen the 'integrated project Bachelor' (see Fig. 1), which constitutes the schnapps project, which is an elective. This small number meant some extra effort for each student, but since everything had been properly set up last year, this was manageable. The students selected pears as starting material. It was quite some effort to produce the mash from 150 kg of pears, which had to be cleaned and cut in advance. As every year, the students put a lot of effort in designing and performing the distillation step. This means that they need to acquaint themselves with the Rayleigh equation before this is taught in the lectures. Everything went well and a delicious product has been obtained, of which not a single drop was wasted (see Fig. 2)

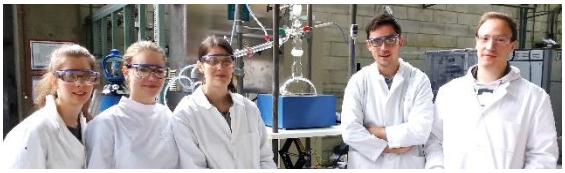

Fig. 1: The schnapps team in front of the still

The project concluded with an appropriate ceremony, where the students first presented their results and their formal documentation, which is the description of the schnapps project on our website. On that website the final presentation is also available, which is especially interesting, because the students recorded their voices, so that the actual presentation is preserved: You are welcome to watch. As a basis for the tasting of the project products, the students had prepared some dishes for the party. After tasting the product, evaluating it, and based on that deciding the grades, the certificates were handed over as shown in Fig. 3. Finally it should be mentioned that the schnapps project meanwhile has already made its appearance in the media, namely in an interview at the BRF, the German-speaking radio broadcasting in Belgium.

The advantage of being so few students was of course that the amount of product per student was considerable. This will change for coming year, where 14 students inscribed.

Fig. 2: Tasting the product: don't waste a single drop of the precious fluid

Fig. 3: The team with certificates and Dr. Laurent Fraikin, who supported, in front of creative and elegant project logo

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An up to date list of publications is available at: http://orbi.ulg.ac.be/ph-search?uid=U222548

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