Process Intensification of Liquid Liquid Systems

Work Package 2: Modelling and process description

Aims of Work Package 2

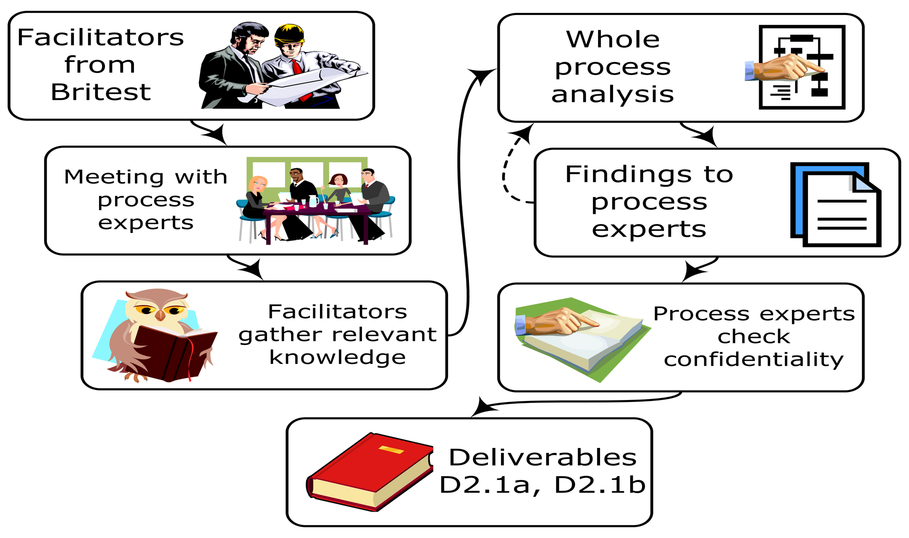
To develop and use mathematical modelling and numerical simulations to understand the interactions between all phenomena and sub-processes involved in the liquid-liquid dispersed phase reactions in structured equipment, to ensure successful design of manufacturing processes and proper interpretation of related experimental data.

(WUT, BRI, EPF, FCTUC, GIV, CUF, FLU, HUN, IMM)

Task 2.1
Studies of the whole process design of the process from the bulk organic chemicals sector and design aspects of the multipurpose plant (coordinated by Britest)

2.1a

- A summary of the information about the process from the bulk organic chemicals sector is given based on public literature and commercial processes operated by PILLS partners.
- An analysis of the knowledge gaps an opportunities for process improvement is presented; this includes increase of yield and improvement of the reaction selectivity.
- Alternative methods of making the product are analysed.
- Recommendations for work on improving the process understanding are presented.



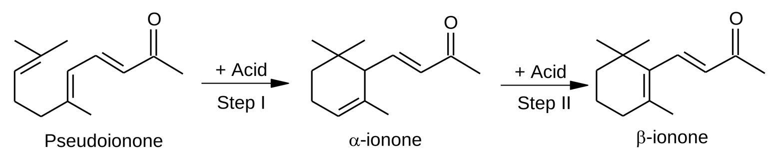
2.1b

The work on the whole process analysis of the β-ionone process is related here to development of a generic whole process design methodology for systems that can involve a liquid-liquid two-phase reaction.

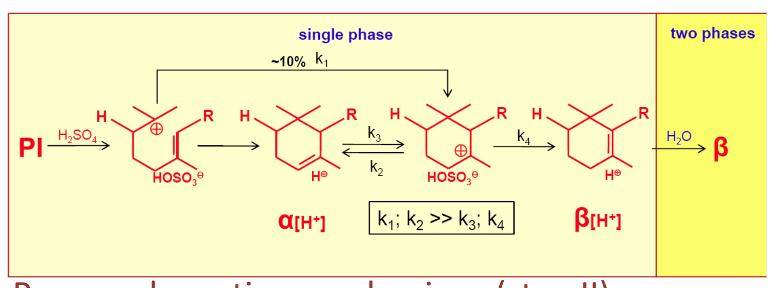
Task 2.2
Determination of kinetics for considered processes

2.2a Cyclisation of pseudoionone (coordinated by Givaudan).

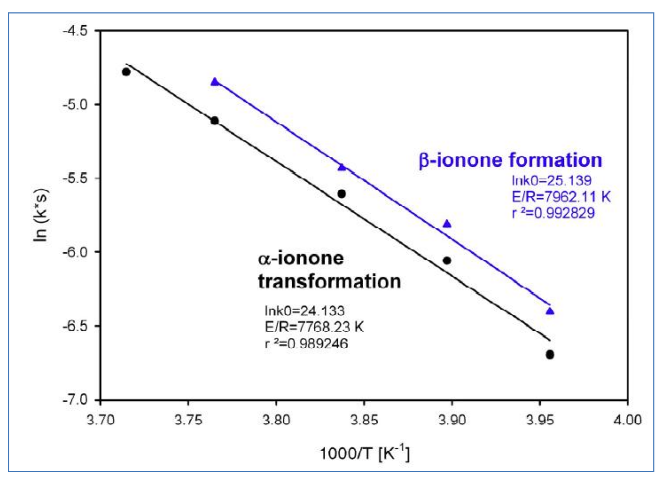
The reaction (cyclisation of pseudoionone (PI) to β-ionone) takes place in acid phase and the product transfers into the organic phase upon dilution of acid with water. Cyclisation of PI to α-ionone (step I) is almost instantaneous, kinetics of step II should be considered in detail.

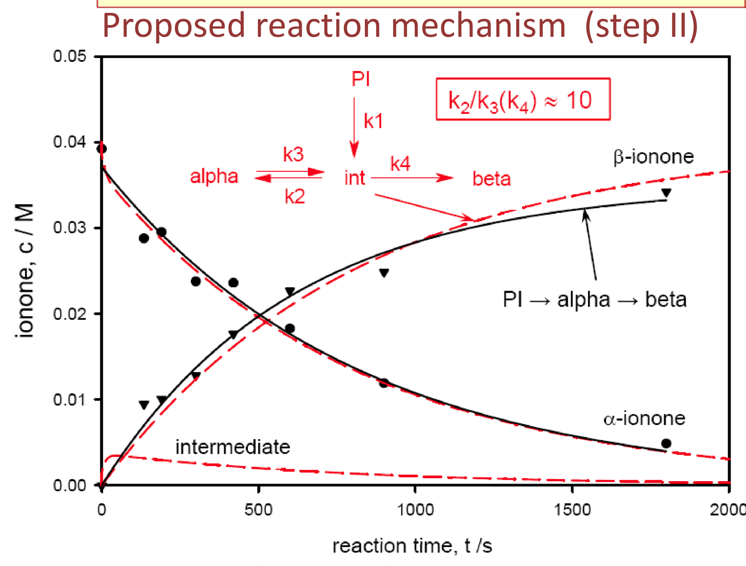


Isomerisation of α-ionone to β-ionone (II step)



Proposed reaction mechanism (step II)





Arrhenius plot for isomerisation reaction (up) and results of fitting to experimental data (right).

2.2b Determination of kinetics for the process from the bulk organic chemicals sector (coordinated by FCTUC).

The work is in progress. The set-up with a micromixer coupled to a tube/reactor to increase the residence time is applied.

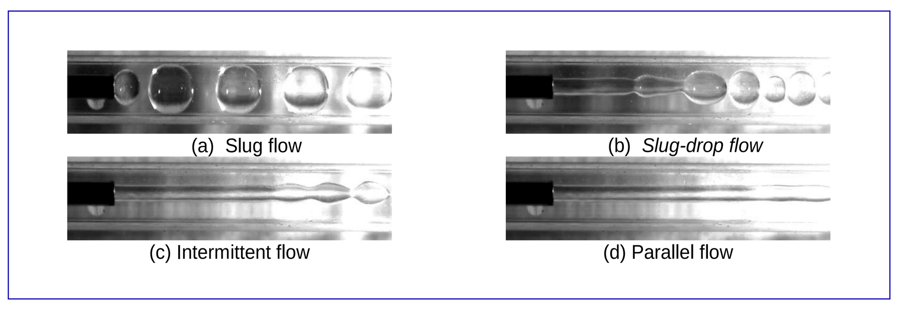
Task 2.7
Model validation(coordinated by WUT)

Models developed in tasks 2.5 and 2.6 will be validated in respect to experimental data.

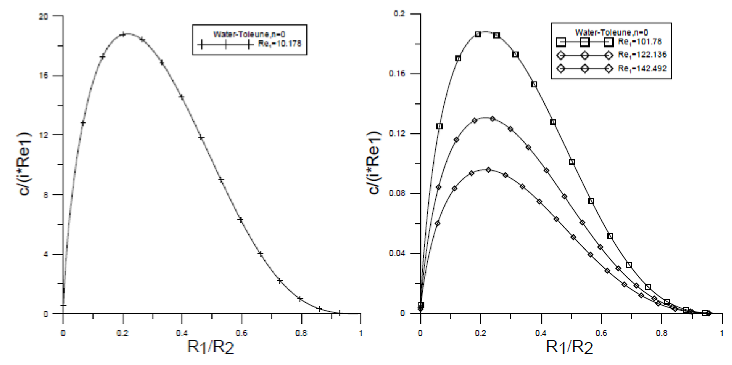
Task 2.8
Final analysis of whole process design (coordinated by FCTUC)

Task 2.3
Determination of flow pattern in micro reactors (coordinated by IMM)

Systematic experimental determination of different flow regimes in single microchannels (slug flow, parallel flow, annular flow etc.) allow for an *a priori* prediction of the different patterns. The theory of linear stability is used to interpret experimental observations.



Flow regimes observed in two phase concentric reactor (water – toluene) for equal flow rates of both phases.

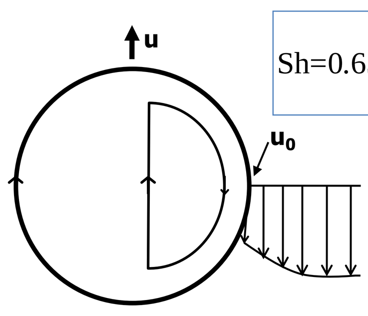


Predictions of perturbation rate

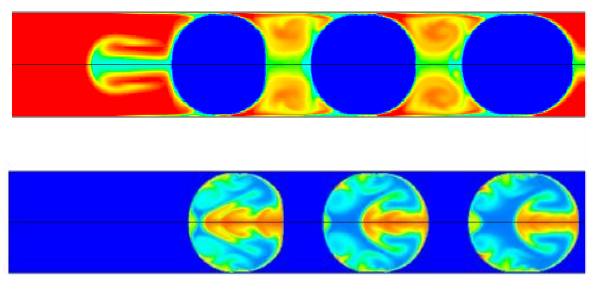
The results are performed to be used into the reactor development.

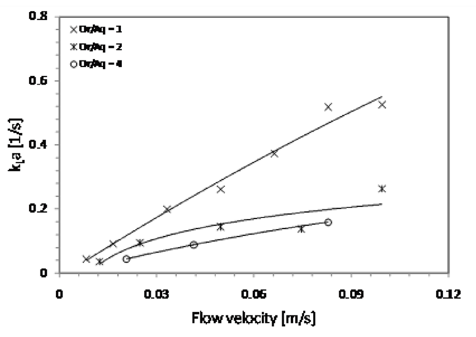
Task 2.4
Determination of mass transfer for different devices and flow pattern (coordinated by EPFL)

The investigation of accurate mass transfer coefficients is a challenging task as in most of the microreactors, the time required for separation of two phases is higher that their contact time in the reaction zone. Effects of operating conditions such as flow velocity, reactor dimensions and physical properties of the systems on the mass transfer characteristics are studied.



$$Sh=0.65\left(\frac{\mu_c}{\mu_d+\mu_c}\right)^{1/2} Pe^{1/2}$$

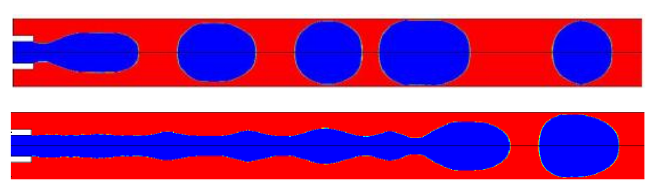




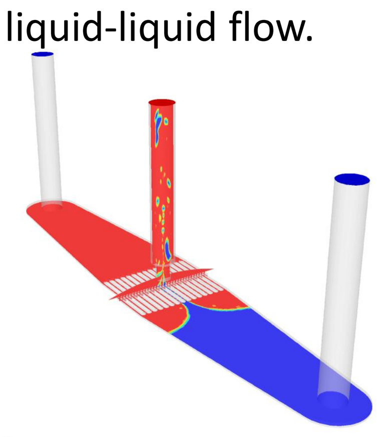
Phenomenological models including surface mobility and fluid deformation, and CFD (VOF modelling) are used to predict mass transfer coefficients and compare them with experimental data.

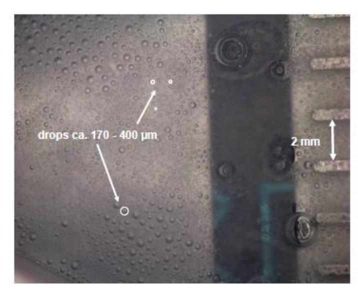
Task 2.5
Generation of CFD models for flow pattern and mixing for devices applied in the project (coordinated by WUT)

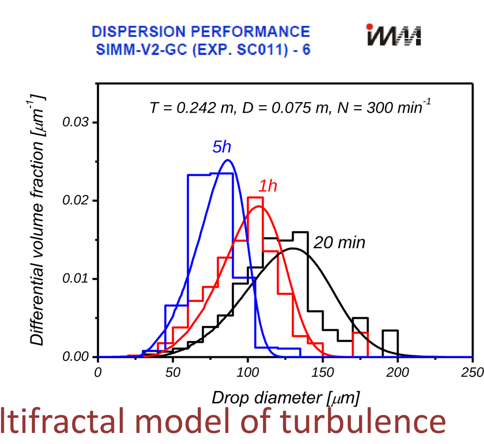
The rational design of micro-structured devices and process modelling require the interpretation of effects of process conditions and reactor geometry of flow pattern and mixing, with the CFD codes for two-phase liquid-liquid flow.

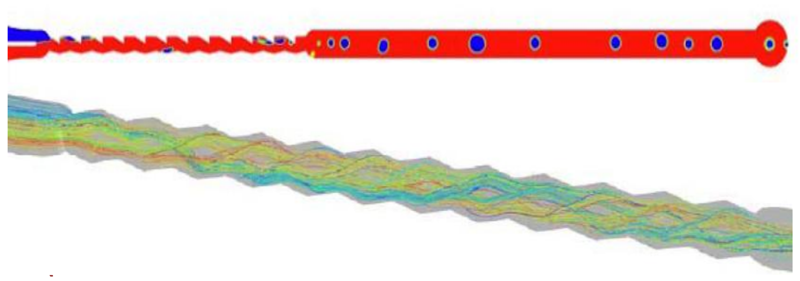


CFD predictions for toluene-water system, Re_1 = 102 and Re_1 = 142 and dispersion in the in mixtrukture-simmv2 (right).

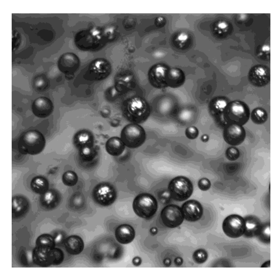








Dispersion and mixing in caterpillar mixer

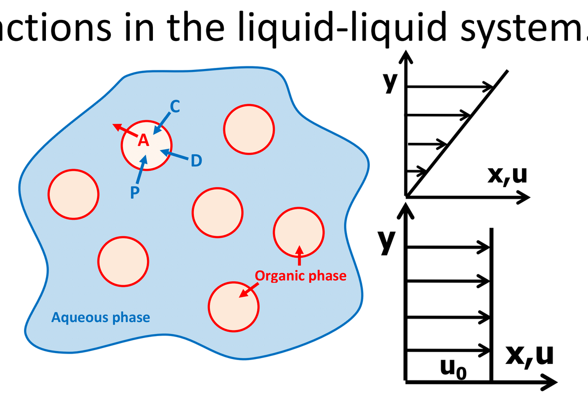


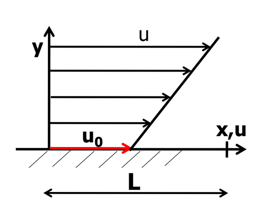
Application of the multifractal model of turbulence

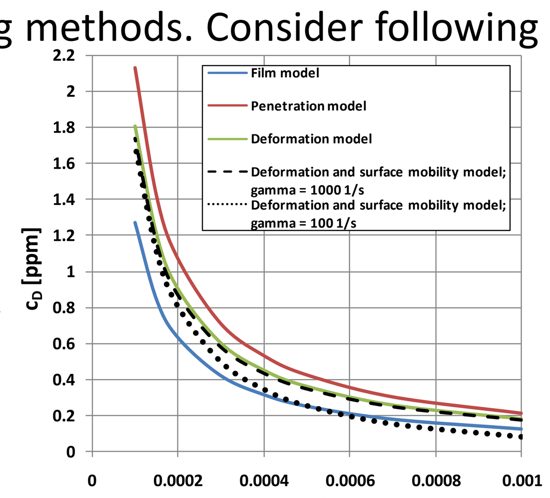
Task 2.6
Multiphase reactor models (coordinated by WUT)

Integration of predictive models using CFD and hybrid modelling methods. Consider following set of complex reactions in the liquid-liquid system.

$$A+B\xrightarrow{k_1}C \qquad (1)$$
$$C+B\xrightarrow{k_2}D \qquad (2)$$
$$A+2B\xrightarrow{k_3}P \qquad (3)$$







Methodology for interpretation of mass transfer with chemical reactions in liquid-liquid systems has been developed for problems of PILLS project.

Effect of flow structure on byproduct concentration

SEVENTH FRAMEWORK PROGRAMME

The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° NMP2-SL-2008-214599