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Liquid-liquid slug flow capillary millireactor

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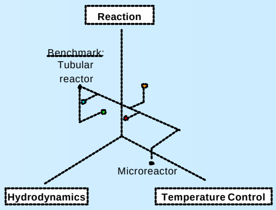
Slug Flow

Advantages

- ⇨ Constant slug volume with well defined mass transfer area
- ⇨ Enhanced mass transfer due to internal circulations within the slug
- ⇨ Better mass transfer leads to reduced process volume and higher reaction rate
- ⇨ Precise control of strongly exothermic and hazardous reactions
- ⇨ Possible technical relevance (?)
- ⇨ Wide applications in phase transfer catalysis, extraction, polymerisation, etc.

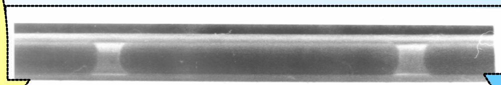
Process Intensification

- ⇨ Key activity in the development of sustainable technology for the chemical industry
- ⇨ Most common chemical processes are limited by reaction, hydrodynamics and/or heat or mass transfer
- ⇨ Intensification enhances these three factors → **Higher yield/selectivity**
- ⇨ Debottlenecking on milli/micro-scale



For two-phase liquid-liquid reaction exhibiting mass-transport-limitations e.g. nitration of single ring aromatics

SLUG FLOW



Problems

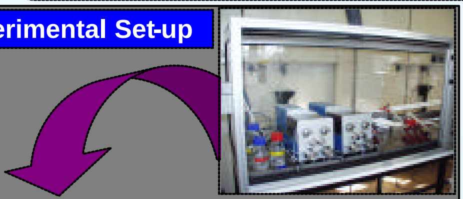
- ⇨ Experimental Slug Flow Stability
- ⇨ Wall Film Stability
- ⇨ Hydrodynamics not completely understood
- ⇨ Selectivity Problem
- ⇨ Influence of Film on circulation

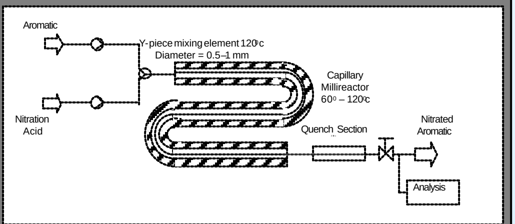
Key Parameters

Pressure drop, **Film thickness**, Circulation patterns, Rate of mixing, Length of aqueous and organic slugs, Mass transfer coefficients

Modelling

Experimental Set-up

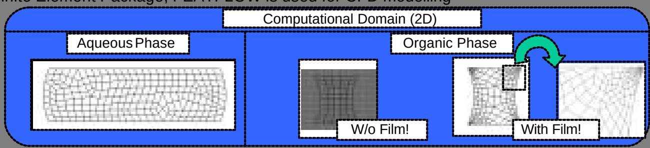




Computational Fluid Dynamics

Problem Details and Solver:

- ⇨ Operating conditions from experiments of Dummann et al (2003)[1]
- ⇨ Using experimental geometry of aqueous and organic slug, solved individual slug as single phase flow
- ⇨ **NO FREE SURFACE MODELLING**
- ⇨ Assumption: Front and back interface of the slug is same
- ⇨ Finite Element Package, FEATFLOW is used for CFD modelling

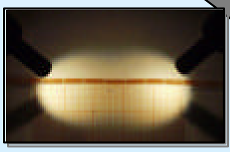


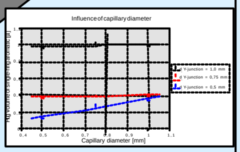
Boundary Conditions:

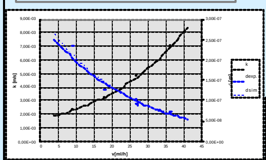
- ⇨ Negative velocity at the wall which moves boundary in reverse direction while interface is kept stationary
- ⇨ Aqueous Slug: Dirichlet type boundary conditions
- ⇨ Organic Slug: Dirichlet type boundary condition for without film while Neumann type for with film

Results

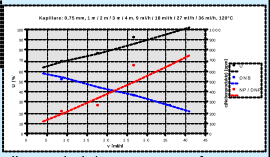
Microscopic Measurements







Influence of flow velocity on mass transfer and film thickness



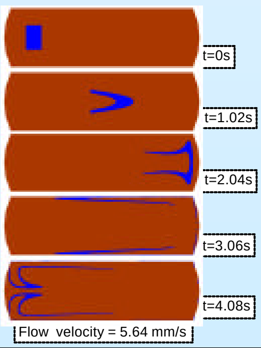
Influence of flow velocity on conversion[1]

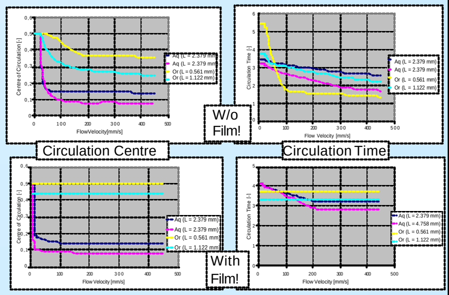
(Ph – Phenolic by-product DN – Dinitrated by-prduct)

- ⇨ Dynamic experiments unexpectedly reveled the presence of an organic wall film of ~ 0.05 mm thickness

Simulations for Internal Circulations

Average circulation time[4] is the time required for liquid particles to move from one end of the slug to the other end





Conclusion

- ⇨ The experimental results shows the slug of constant volume and well defined mass transfer area.
- ⇨ For slug with sufficient length (L>D), film has no significant effect on circulation time
- ⇨ Circulation time decreases with increase in mixture velocity in slug flow without film

Future Work

- ⇨ Develop free surface CFD model for slug flow with film
- ⇨ Experimentation using tracer technique to predict the internal circulations
- ⇨ Study of hydrodynamic parameters such as pressure drop, mass transfer coefficient by physical and numerical experiments

References

1. Dummann et al., The capillary microreactor: a new concept for the intensification of heat and mass transfer in liquid-liquid reactions, *Cat. Today, 79-80, 433-439, 2003.*
2. Gruber Rainer., Radial mass transfer enhancement in bubble train flow, *Ph.D Thesis, RWTH Aachen, 2001.*
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4. Thulasidas et al., Flow patterns in liquid slugs during bubble train flow inside capillaries, *Chem. Eng. Sci., 52 (17), 2947-2962, 1997.*

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