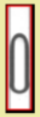
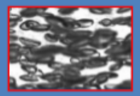
ENTWICKLUNG UND ANWENDUNG EINER METHODE ZUR DIREKTEN NUMERISCHEN SIMULATION REAKTIVER TRANSPORTPROZESSE IN BLASENSYSTEMEN

Dennis Hillenbrand, Holger Marschall

STRUCTURE SPP 1740

	complexity methods	***SuperFocusMixer***  *coordination:* *S. Schindler*	***Taylor Flow***  *coordination:* *G. Rinke*	***Bubble Swarms***  *coordination:* *H. Marschall*	***Bubbly Flows***  *coordination:* *U. Hampel*
A	Experiments *coordination: M. Schlüter*	M. Schlüter G. Rinke/W. Simon	U. Hampel **G. Rinke/W. Simon** M. Schlüter	**M. Kraume** **M. Schlüter** G. Rinke/W. Simon	**C. Brücker** **U. Hampel** **C. Kähler** **J. Thöming**
B	Simulation and modeling *coordination: D. Bothe*	**S. Turek**	D. Bothe H. Marschall S. Turek	**D. Bothe** **H. Marschall**	**R. Rzehak** **M. Hlawitschka**
C	Chemistry reaction networks *coordination: S. Herres-Pawlis*	**S. Herres-Pawlis** **P. Klüfers** G. Rinke/W. Simon **S. Schindler**	G. Rinke/W. Simon S. Schindler S. Herres-Pawlis **D. Ziegenbalg**	S. Schindler S. Herres-Pawlis	P. Klüfers
D	Transfer to selective reactions in bubbly flows *coordination: U. Nieken*			M. Hlawitschka	**M. Hlawitschka** **U. Nieken** **U. Tuttlies** **K. Zähringer**

SCIENTIFIC RELEVANCE

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Review Article

Review on hydrodynamics and mass transfer in minichannel wall reactors with gas–liquid Taylor flow

CrossMark

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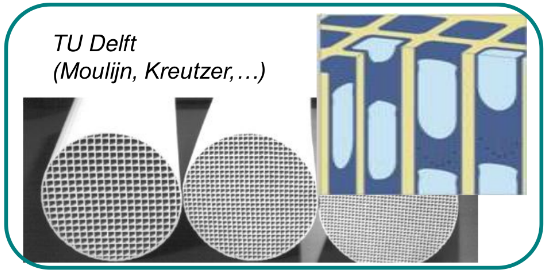
Dedicated to Prof. Dr.-Ing. habil. Rüdiger Lange on the occasion of his 65th birthday.

"The reviewed literature identifies no clear window of operating conditions and hydrodynamic parameters at which Taylor flow offers the highest mass transfer"

INDUSTRIAL RELEVANCE

- Used for microfluidic applications
- High mass and heat transfer rates
- High mixing rates within liquid slugs
- Controllable flow characteristics



NUMERICAL CHALLENGES

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- Resolution of species boundary layer
- Resolution of wake structures

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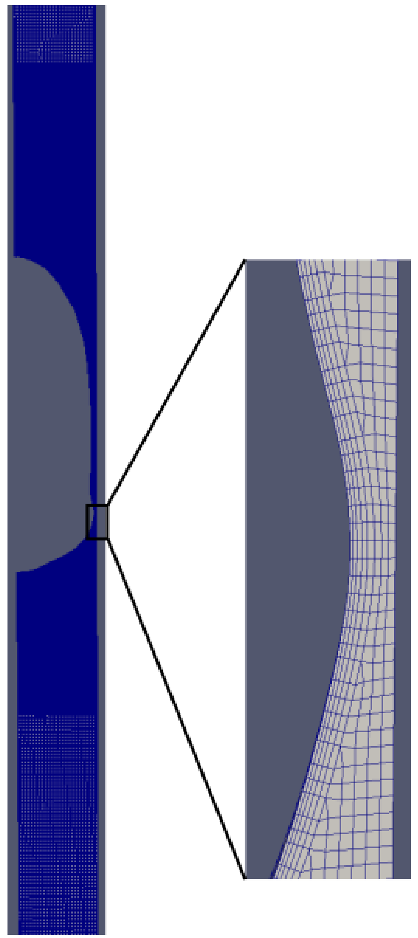
Results in very fine meshes with many cells!



Mesh resolution for Taylor bubble

REDUCED COMPLEXITY

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Experiments and simulations show rotational symmetric hydrodynamics for $Re < 200$

Highly resolved simulations possible for quasi-2D domains

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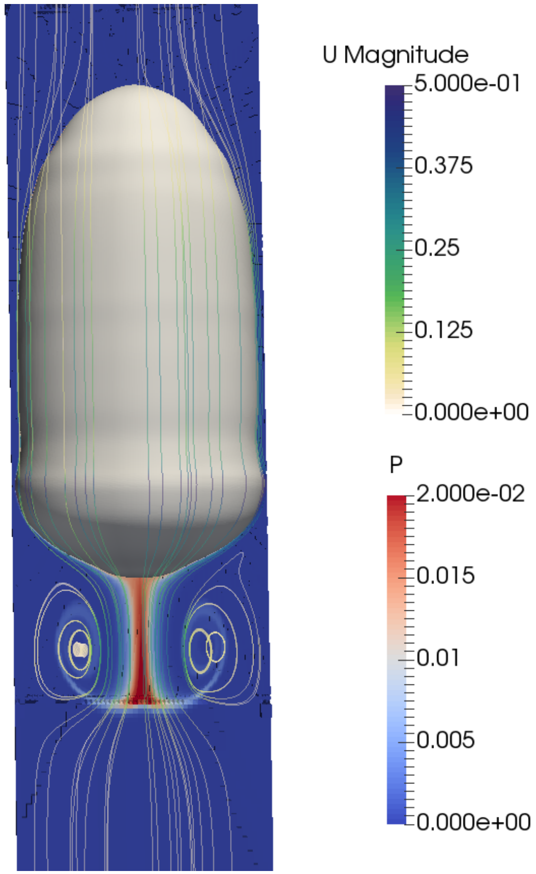


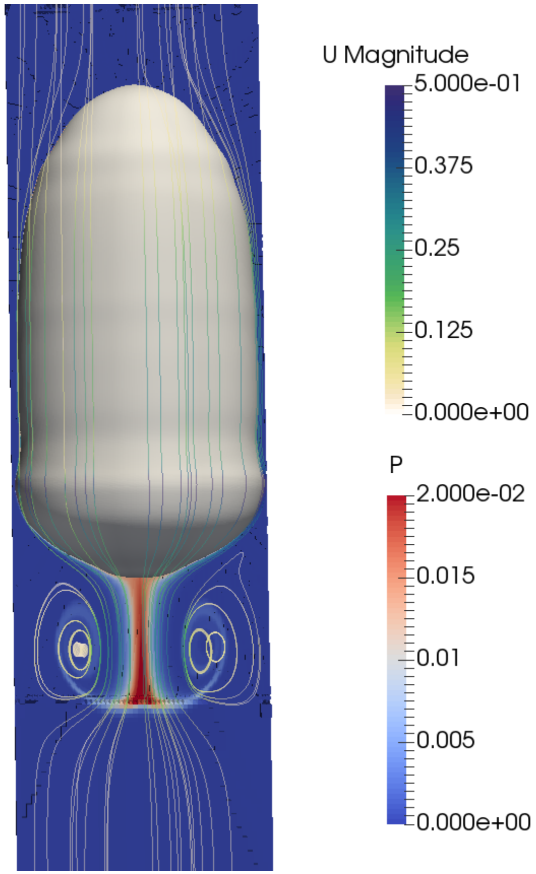
3D study of mass transfer around Taylor bubble

REDUCED COMPLEXITY

Experiments and simulations show rotational symmetric hydrodynamics for $Re < 200$

Highly resolved simulations possible for quasi-2D domains

BUT : Rotational symmetry not accessible in interface tracking simulations!

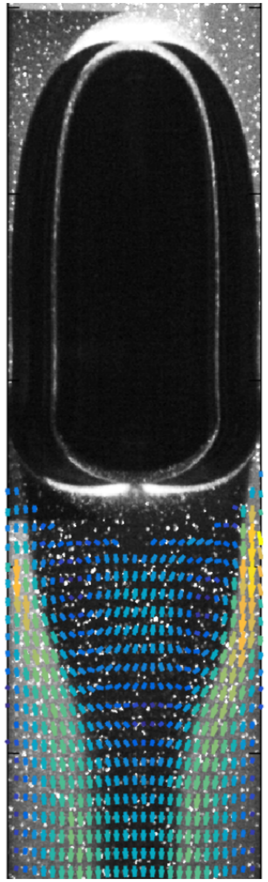


3D study of mass transfer around Taylor bubble

THREE GOALS FOR TAYLOR BUBBLES

1. VALIDATION AGAINST EXPERIMENTS
2. INVESTIGATION OF LOCAL SELECTIVITY
3. MASS TRANSFER CORRELATIONS

1. EXPERIMENTAL VALIDATION



Experimental results, TUHH

bubble shape

rise velocity and
flow patterns

Numerical simulation

2. LOCAL SELECTIVITY

Competitive consecutive schemes

$$A + B \xrightarrow{k_1} P$$

$$A + P \xrightarrow{k_2} S$$

Realistic and important parameter ranges for reaction ratios $\kappa = \frac{k_2}{k_1}$

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$$A + B \xrightarrow{k_1} P$$

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Realistic and important parameter ranges for reaction ratios $\kappa = \frac{k_2}{k_1}$

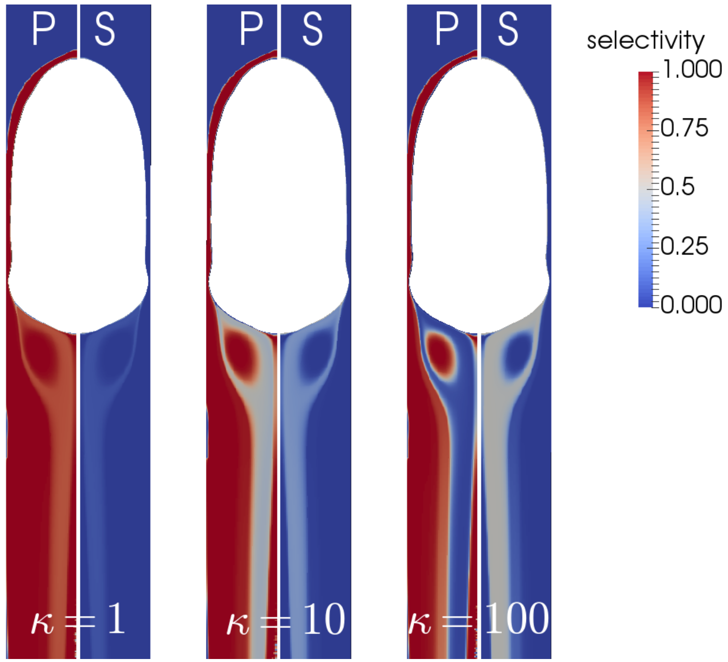
Important parameter: local selectivity

$$Sel_{P,A} = \frac{r_1 - r_2}{r_1 + r_2} = \frac{c_B - \kappa c_P}{c_B + \kappa c_P}$$

2. LOCAL SELECTIVITY

Influence of wake structure on local selectivity

Side product mainly produced along vortex structure
Product selectivity reduced along vortex structures



Selectivity for $Da_1 = 1$

3. MASS TRANSFER CORRELATIONS

- Correlations available in literature for physisorption

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3. MASS TRANSFER CORRELATIONS

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  - Mainly for smaller channels $d \leq 2mm$
  - Mainly applicable in a short range of characteristic parameters
  - Taylor flow can reduce mass transfer due to saturation in the film between bubble and wall
- **No** correlation for enhancement by reaction in bulk phase found

NEXT STEPS

- Validate hydrodynamics against experimental results (TUHH)
- Estimate parameter range with simplified setup
- Two-phase simulations with
  - highly resolved meshes
  - maschine learning SGS model
- Gain insight into local selectivity fields
- Obtain mass transfer correlations including reactions

THANK YOU
FOR YOUR ATTENTION!

REMAINING QUESTIONS?