Multiphase Structured Reactors

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Your energy. Our passion.

Multiphase Structured Reactors

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EPIC5, Nice
1st October, 2015

www.ecn.nl

Our PI solutions for separations

limitation	*solution*	*our technology*
heat transfer limited	heat integrated separation	HIDiC
low temperature	H_2 separation membranes	Hysep
relative volatility	pervaporation membranes	Hybsi
temperature swing solvent	pressure swing sorbent	Alkasorb Plus

Our PI solutions for reactors

limitation	*solution*	*example*
mass & heat transfer	structured reactors	TFR, SMR
intrinsic kinetics	advanced catalysts	syngas, N_2O
thermodynamic	separation enhanced	SEWGS, H2MR

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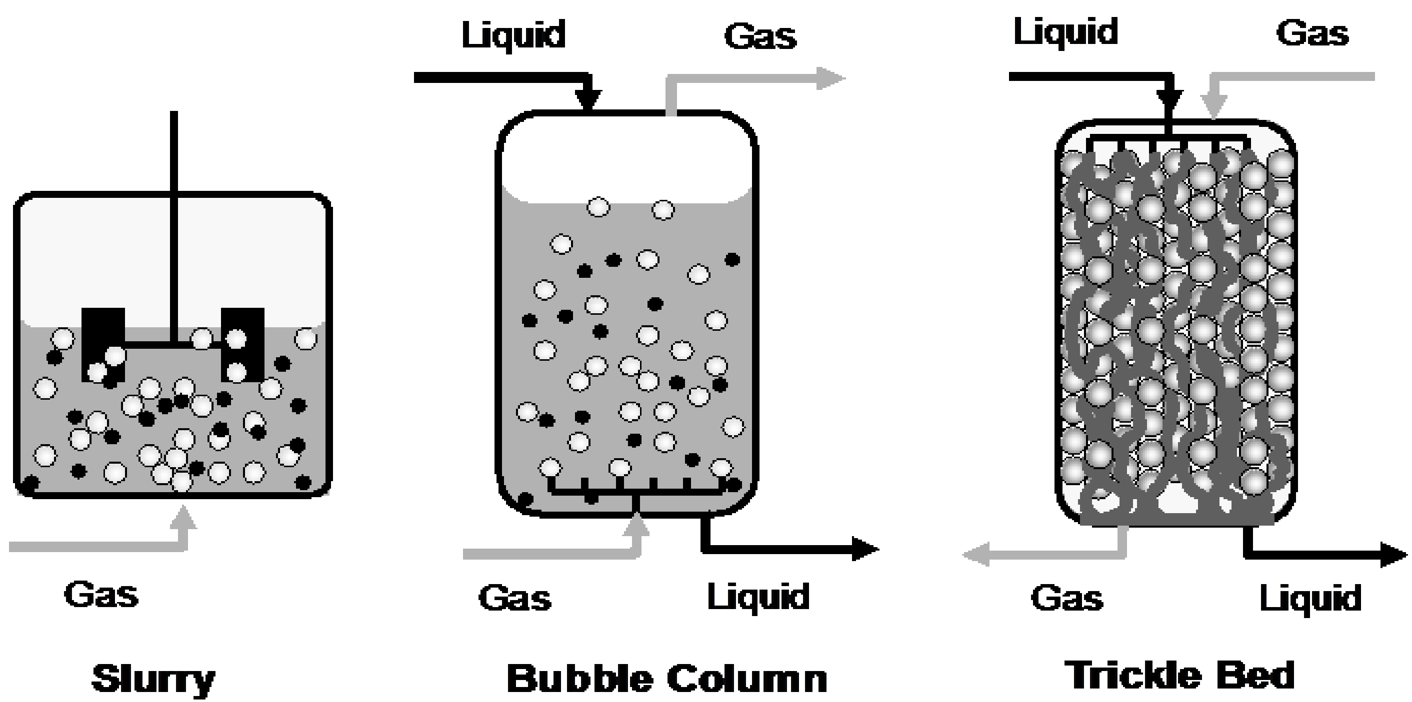
Conventional Gas-Liquid Reactors



Drivers for Structured Reactors

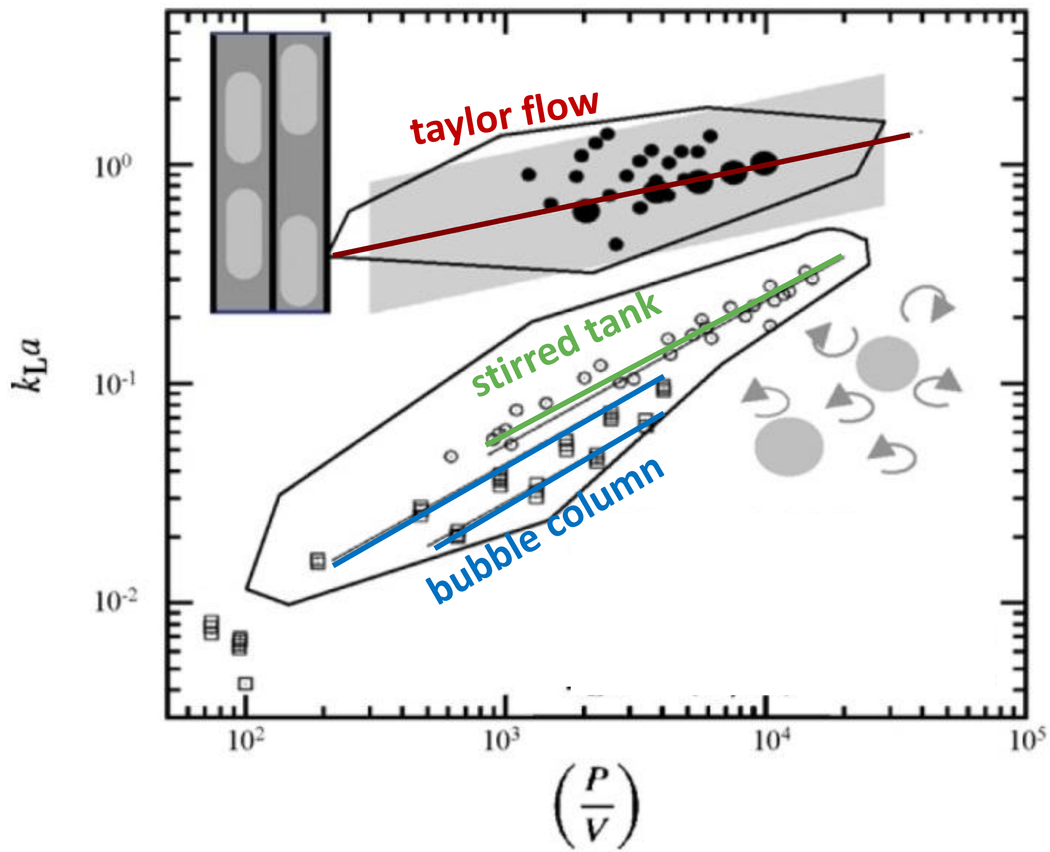
- increased mass transfer
- all reactant undergoes same processing

→ higher conversion
→ higher selectivity

- scale out vs scale up

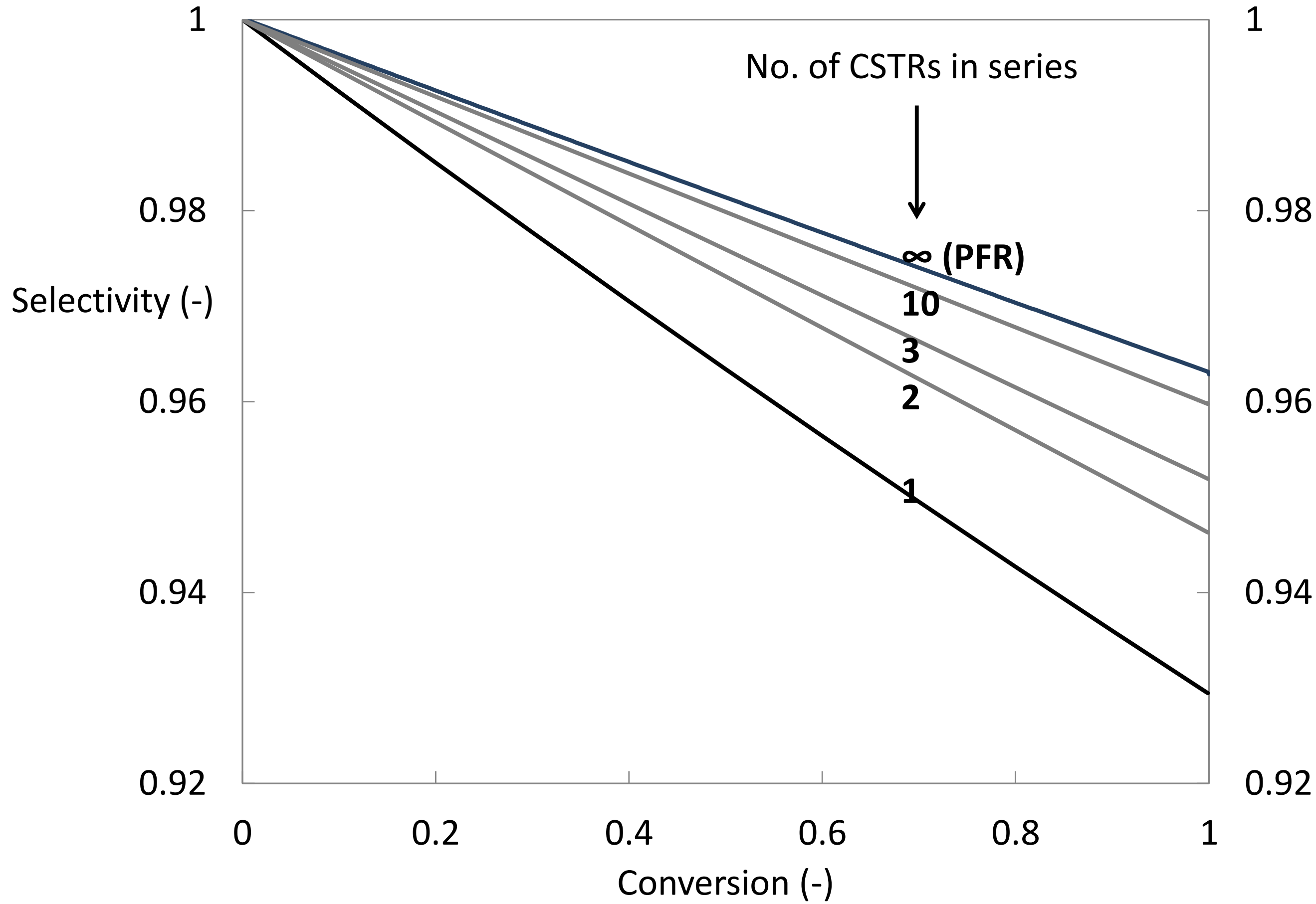
→ predictable performance

Mass Transfer Highest for TFR

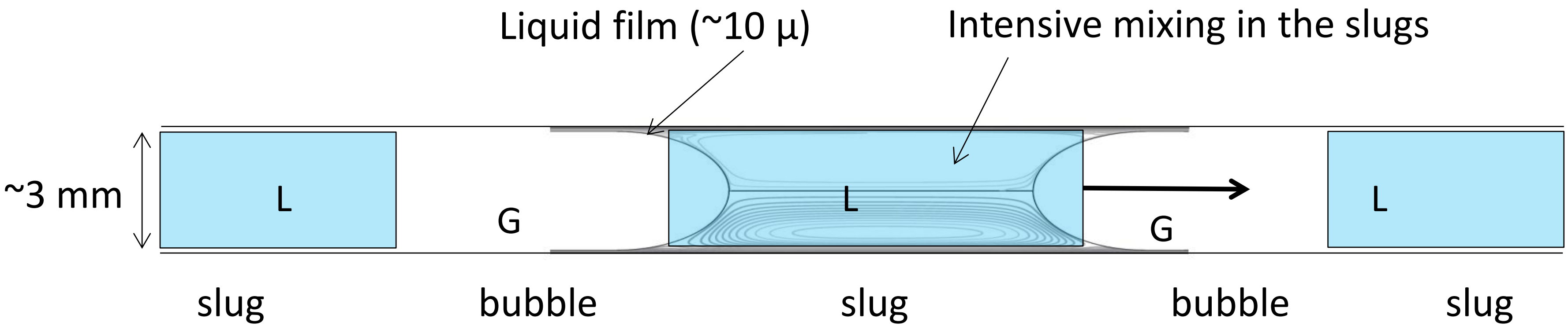


Adapted from: Kreutzer et al. *Catal Today* 111 (2006) 111.

Effect of Residence Time Distribution (RTD) on selectivity



Taylor flow reactor (TFR)



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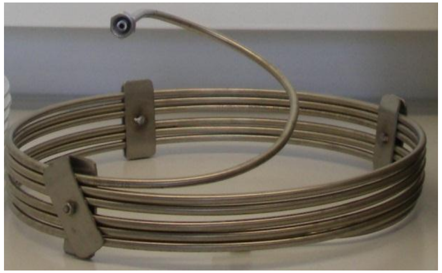
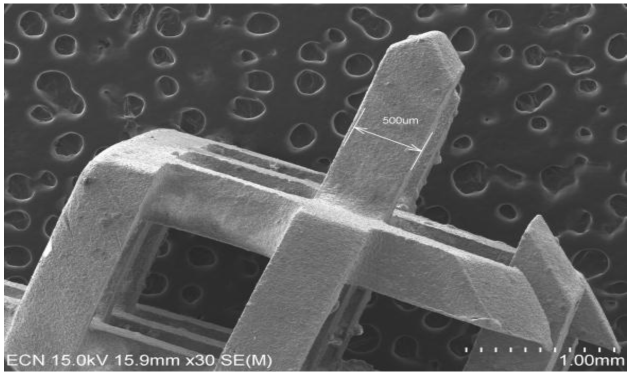


Single pass reactor

Static Mixer Reactor (SMR)



The Project Objectives

To design a flexible gas/liquid reactor based on widely accepted technology … using structured elements within the tubes of the reactor to achieve the required mass and heat transfer properties.

To accelerate the introduction of structured reactors in industry

The model reaction

$B3 + H_2 \rightarrow B2$ (r_1)

$B2 + H_2 \rightarrow B1$ (r_2)

B3: 2-butyne-1,4-diol

B2: 2-butene-1,4-diol

B1: 2-butane-1,4-diol

Kinetic model

Chaudhari et al. *Appl. Catal.* **1987**, *29*, 141

$$r_1 = \frac{w k_1 C_{H2}}{1 + K_{B3} C_{B3}^2}$$

$$r_2 = \frac{w k_2 C_{H2} C_{B2}}{1 + K_{B3} C_{B3}^2}$$

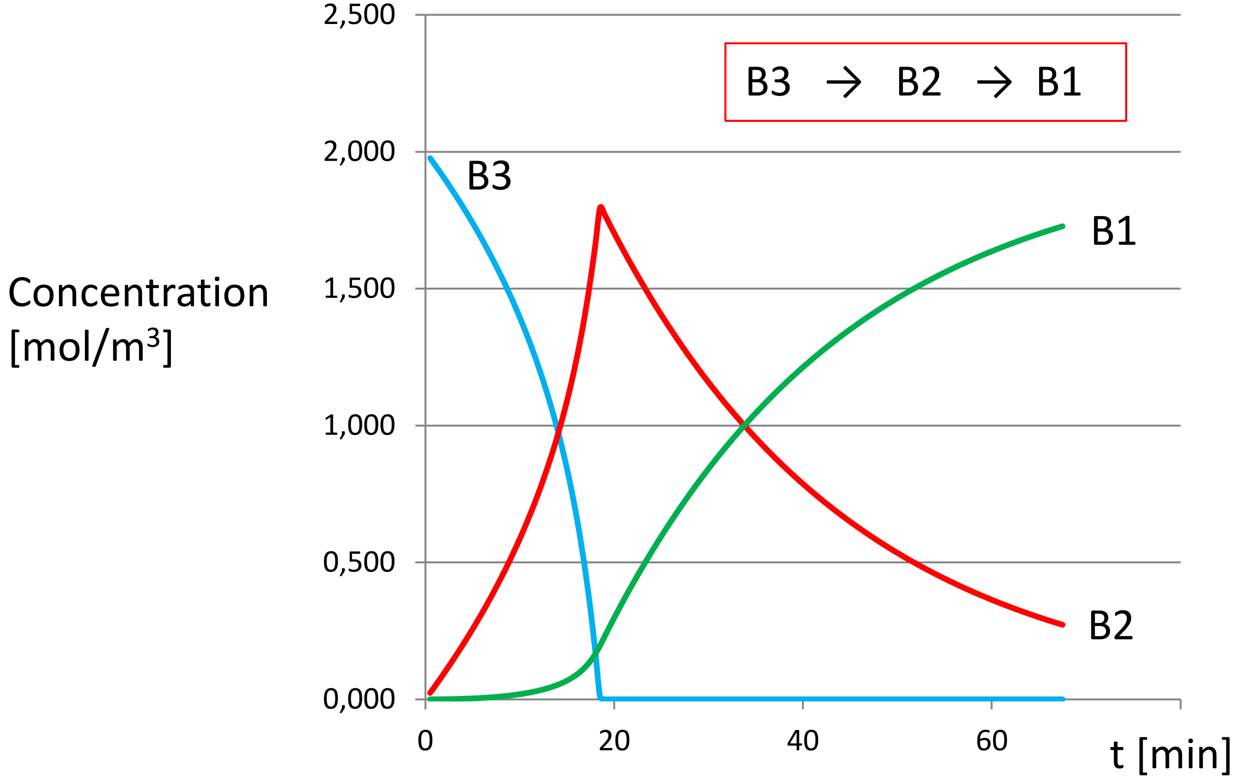
C_i- concentration of i on the catalyst surface, kmol/hr

k_1, k_2 - reaction rate constant, $m^6/(kmol \cdot s \cdot kg_{Pd})$

K_{B3} - adsorption constant of B3, $m^3/kmol$

w – catalysts loading, kg_{Pd}/m^3

Sequential production of B2 and B1



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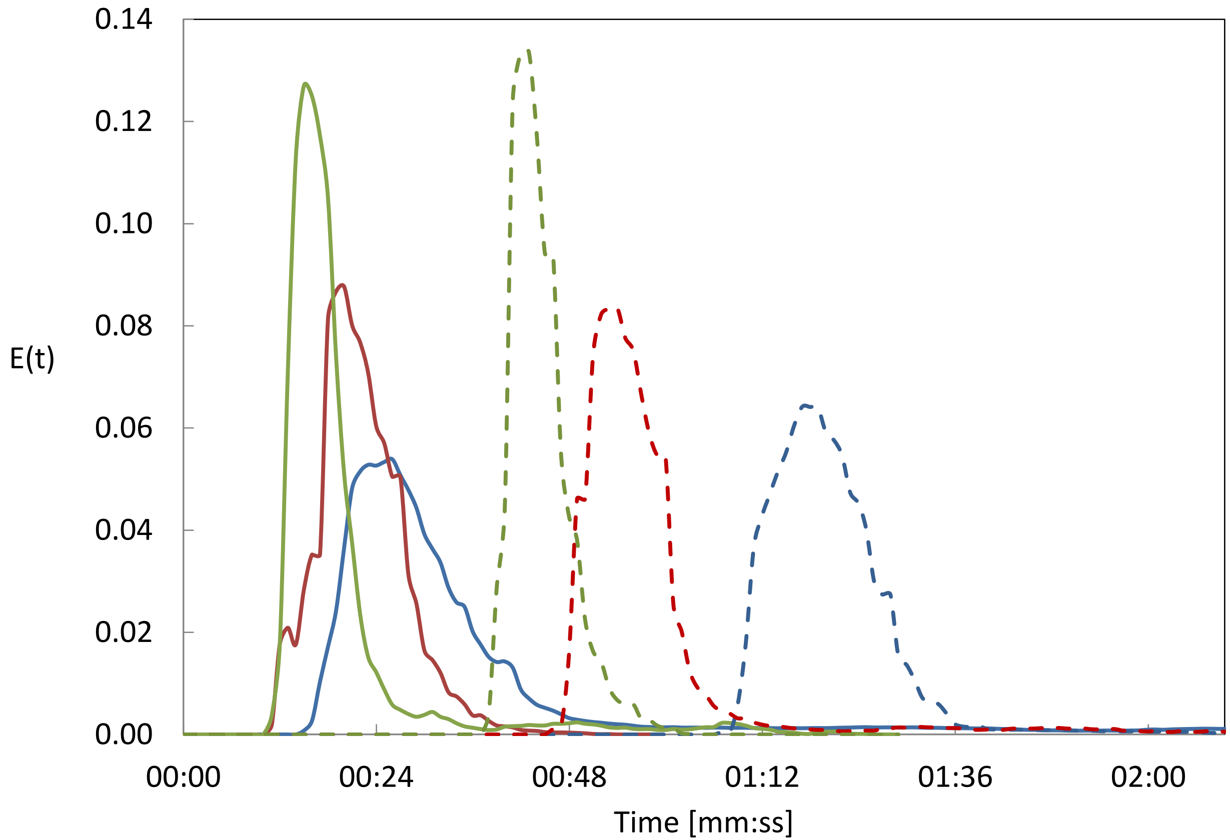
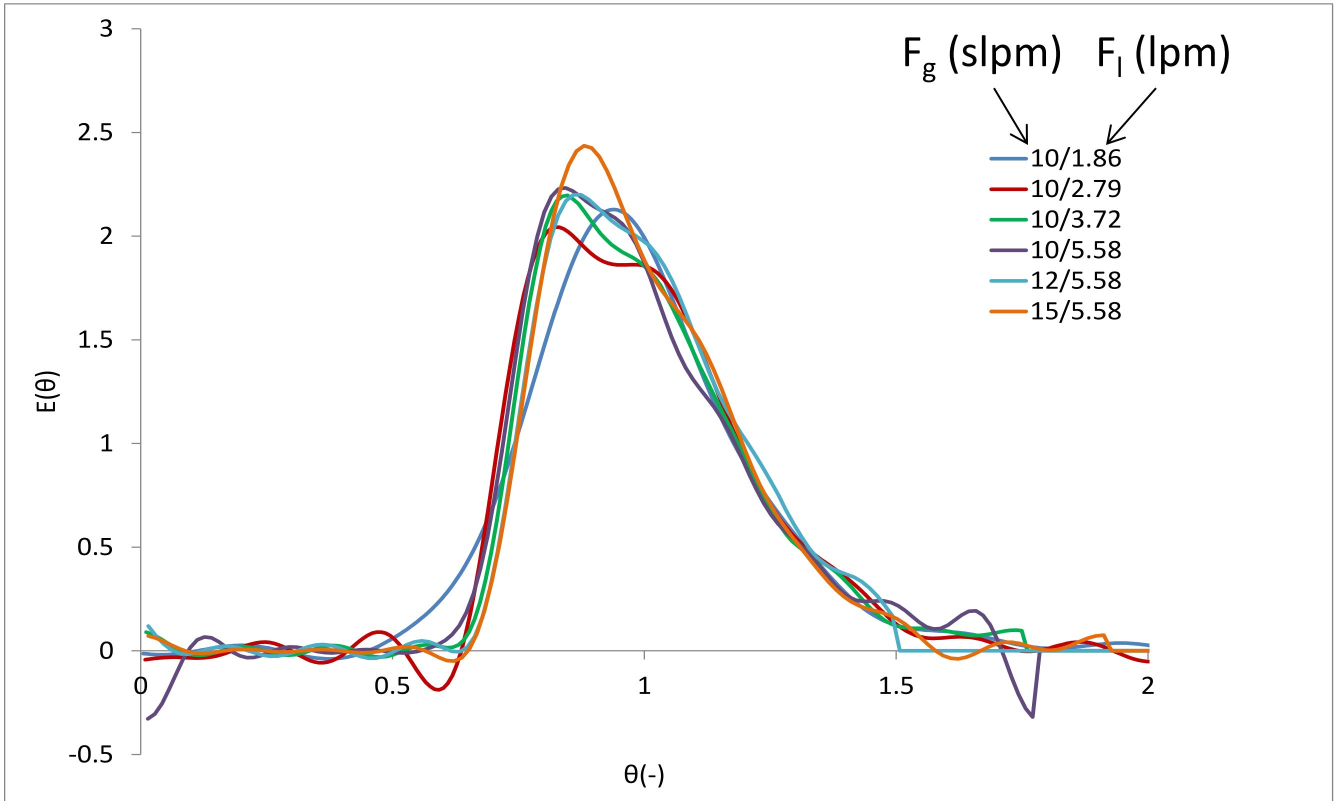
Nearly ideal plug flow in Taylor Flow Reactor



SMR: measured RTD (F_g, F_L)



T ambient

P atmosheric

30% IPA

Pe and N

	$\sigma_{213smx}^2/t_{213smx}^2$	N	Pe	D (m²/s)
1.86 ml/min L, 10 ml/min G	0.0474	21	41	$1.4\cdot10^{-4}$
2.79 ml/min L, 10 ml/min G	0.0331	30	59	$1.7\cdot10^{-4}$
3.72 ml/min L, 10 ml/min G	0.0441	23	44	$2.8\cdot10^{-4}$
5.58 ml/min L, 10 ml/min G	0.0236	42	84	$1.9\cdot10^{-4}$
5.58 ml/min L, 12 ml/min G	0.0356	28	55	$3.1\cdot10^{-4}$
5.58 ml/min L, 15 ml/min G	0.0380	26	52	$3.3\cdot10^{-4}$

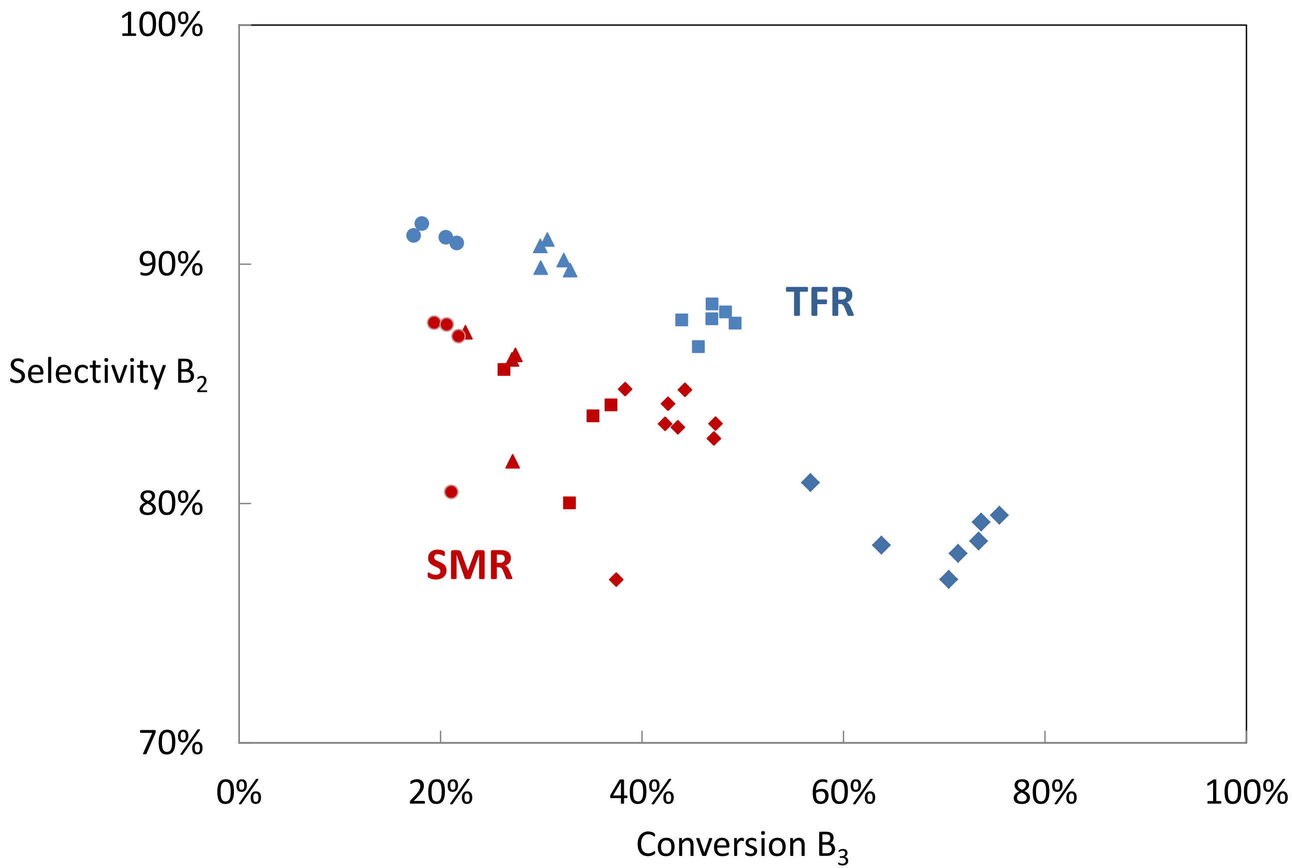
The RTD for *N* ideally mixed tanks in series is given by (Swaaij & Westerterp):

$$E(\theta) = \frac{N^N \theta^{N-1}}{(N-1)!} e^{-N\theta}$$

and its variance is:

$$\frac{\sigma^2}{t^2} = \frac{1}{N}$$

Results: SMX vs TFR



x_{B3} = 3%
T = 22 °C
P = 15 bar

Two reactor models for TFR

Kinetic model for main and side reactions

Chaudhari et al. *Appl. Catal.* **1987**, *29*, 141

Pseudo-homogeneous reactor model

Assumes uniform liquid concentrations in the film in a unit cell

Overall mass transfer gas-liquid-solid

$$k_{GLS}a_{GLS} = k_{GS}a_{GS} + \left(\frac{1}{k_{GL}a_{GL}} + \frac{1}{k_{LS}a_{LS}}\right)^{-1}$$

Kreutzer et al. *Chem. Eng. Sci.* **2005**, *60*, 5895.

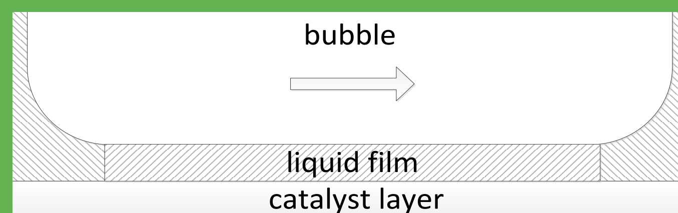
Van Baten & Krishna *Chem. Eng. Sci.* **2004**, *59*, 2535.

Van Baten & Krishna *Chem. Eng. Sci.* **2005**, *60*, 1117.

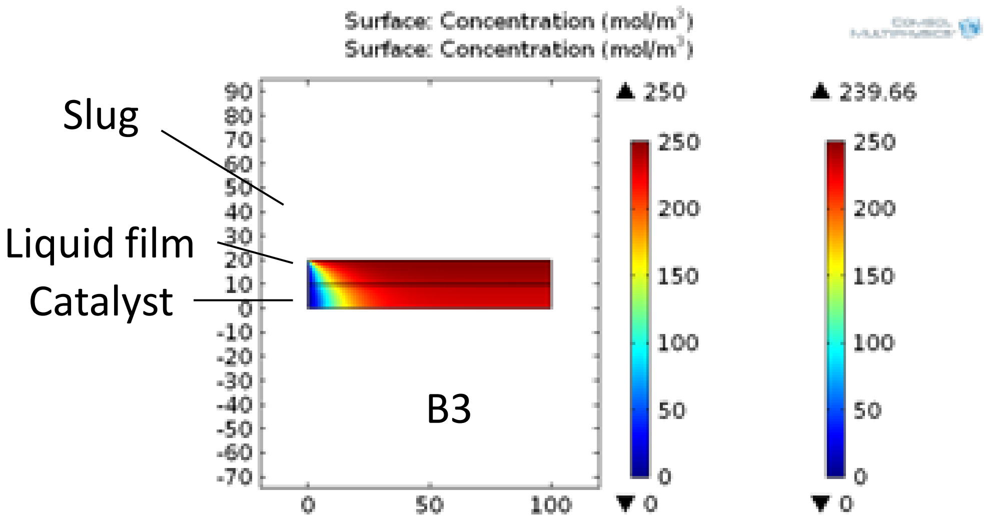
Bubble-and-slug reactor model

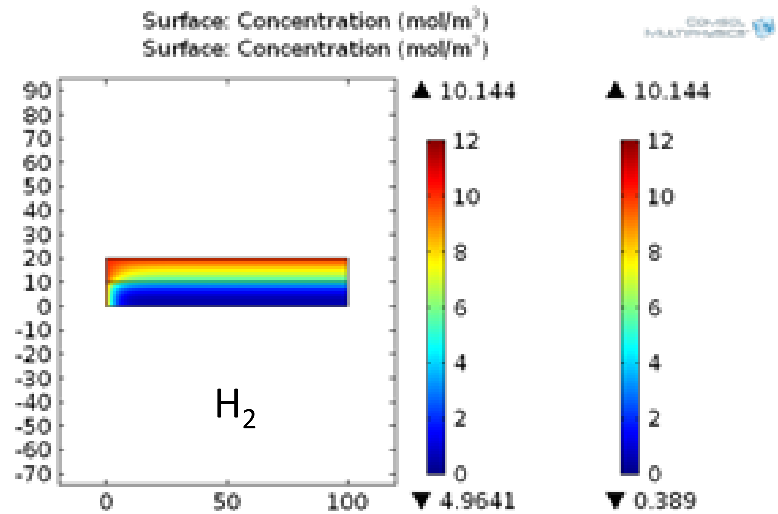
2D axisymmetric diffusion model for liquid film and catalyst layer

Modelling local depletion and replenishment during passing of bubble and slug (transients)



Passing slug

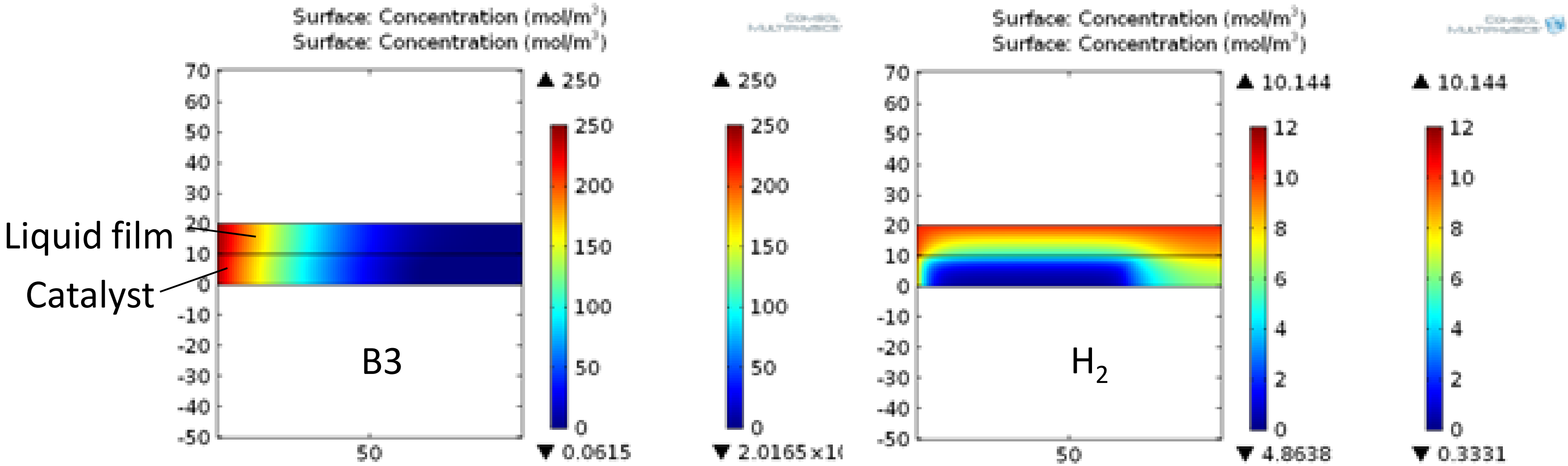




B3 is readily replenished

H_2 concentration low but not depleted

Passing bubble



Even at high B3 concentration in the bulk, B3 present in liquid film and catalyst layer is fully converted during the passage of a bubble

Summary

- The Taylor flow reactor and static mixer reactor can outperform conventional reactors for gas-liquid reactions, due to their intensified mass transfer capabilities and low axial mixing.
- The experimental Taylor flow reactor shows plug flow behaviour.
- Measured selectivities for a model reaction in a Taylor flow reactor and in a static mixer reactor were 80 to 90%.
- Observed performance for TFR better than for SMR, due to higher mass transfer and closer to plug flow.
- Observed conversions and selectivities for a model reaction were lower than expected (95 - 96%).
  - For the TFR, modelling suggests that depletion of B3 could be the cause. Performance is expected to improve for smaller slugs.

Thank you for your attention

The project received Topsector Energy subsidy from the Dutch Ministery of Economic Affairs

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