Development of a computer code for direct numerical simulation of mass transfer phenomena in two-phase flows

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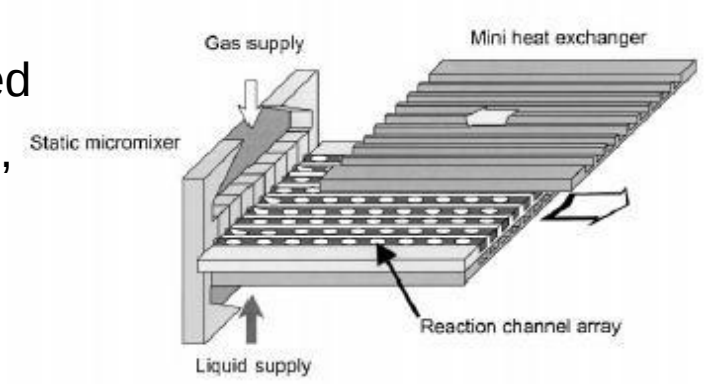
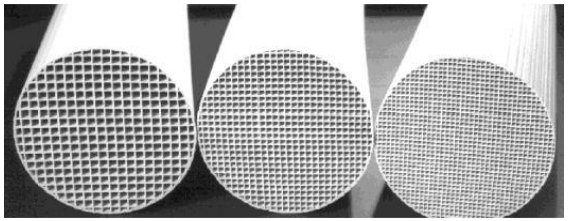
Introduction

- U(VI) extraction in TBP from HNO_3 solutions in a micro-channel within the PUREX process (increased extraction efficiency, reduced amount of waste solutions, increased selectivity)[1]
- Heat/mass transfer in two-fluid flows within mini/micro devices[2]
  - high heat/mass transfer rates due to high interfacial area per unit volume
  - mini/micro devices can operate under more stable conditions and use small amounts of chemicals (increased safety, isothermal flow)
  - well defined flow patterns



Micro Bubble Column



Monolithic Catalyst Reactor

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2. V. Hessel, S. Hardt, H. Löwe – Chemical Micro Process Engineering, 2004

Computer code TURBIT - VoF

- Numerical code developed for simulation of laminar and turbulent flows in one-phase and two-phase flows in plane channels
- Time-dependent conservation equations for mass, momentum and energy of two incompressible, immiscible fluids
- Volume-of-Fluid technique for interface tracking
- Transport equation for the liquid volumetric fraction
- Periodic boundary conditions in flow direction

Governing equations

- Species conservation equation:

$$\frac{\partial c_k^\alpha}{\partial t} + \nabla \cdot \left(c_k^\alpha \mathbf{v}_k \right) = -\nabla \cdot \mathbf{j}_k^\alpha + r_k^\alpha, \quad k = 1, 2$$

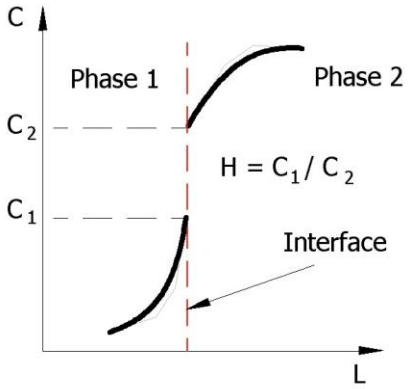
- Fick's law: $\mathbf{j}^\alpha = -D^\alpha \nabla c^\alpha$
- Interfacial constitutive equation: $\mathbf{j}_1^\alpha \cdot \mathbf{n} = \mathbf{j}_2^\alpha \cdot \mathbf{n}$
- Interfacial local equilibrium instantaneously established (Henry's law):

$$H^\alpha = \frac{c_1^\alpha}{c_2^\alpha}$$

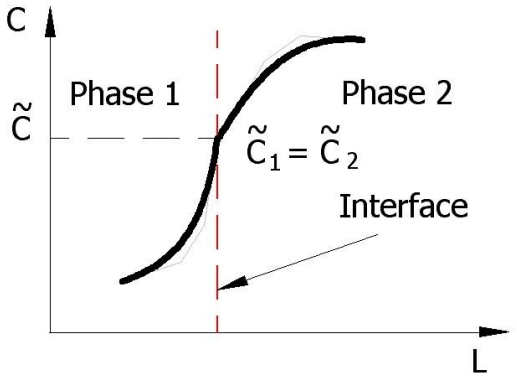
c_1^α – concentration of species α in the liquid

c_2^α – concentration of species α in the gas

- Concentration field is transformed to ensure continuity

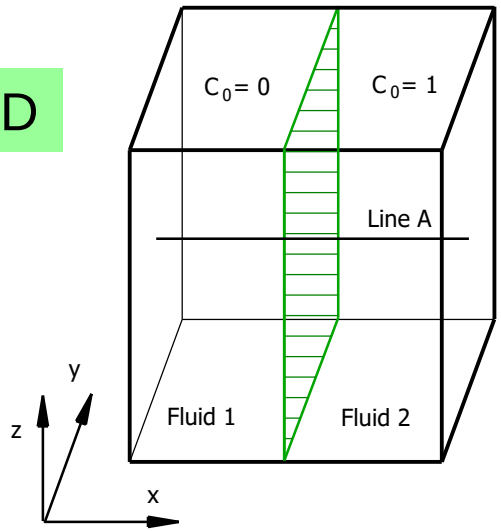


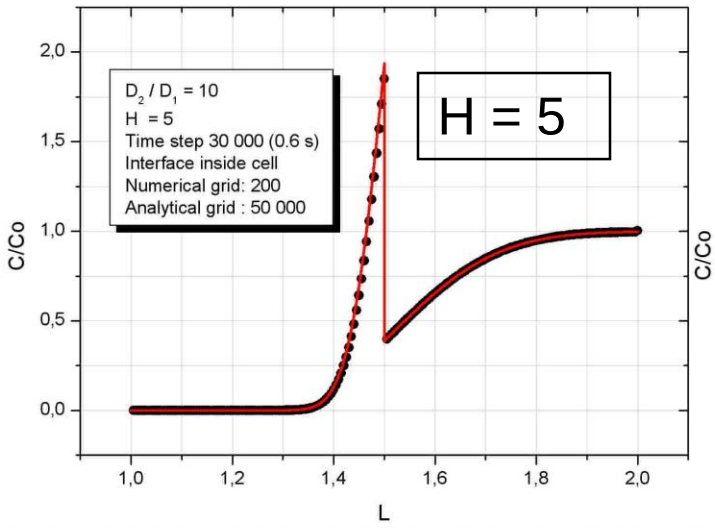
$$\tilde{c} = \begin{cases} c_1^\alpha, & \text{phase 1} \\ H^\alpha c_2^\alpha, & \text{phase 2} \end{cases}$$

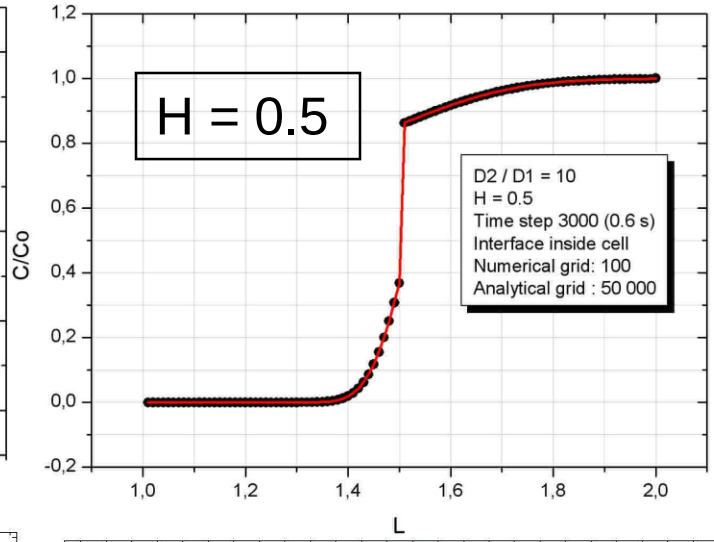


Validation of the diffusive term

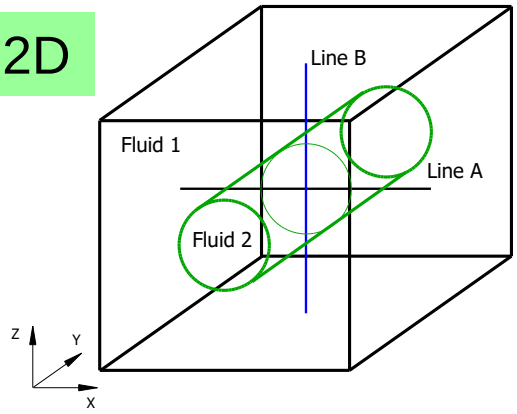
1D

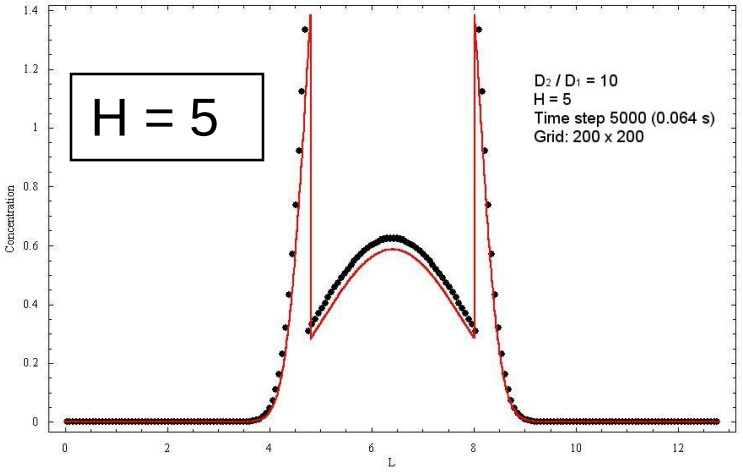


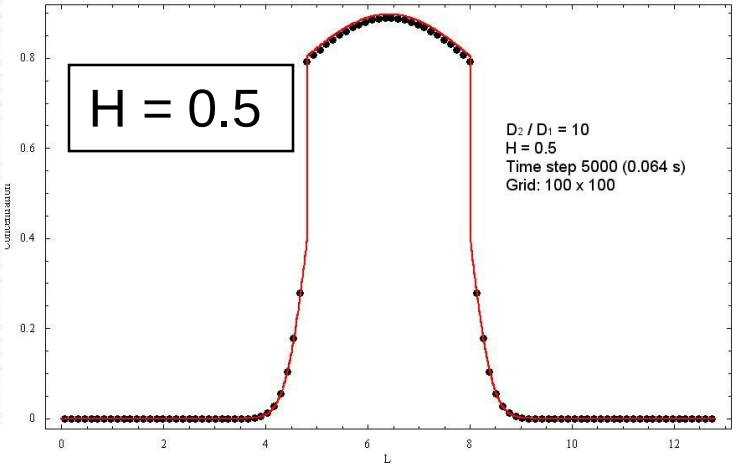




2D







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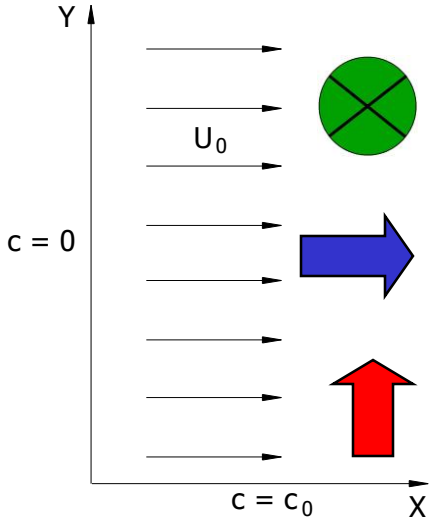
Validation of the source term

Mass transfer with first order homogeneous and heterogeneous reaction in single phase flow

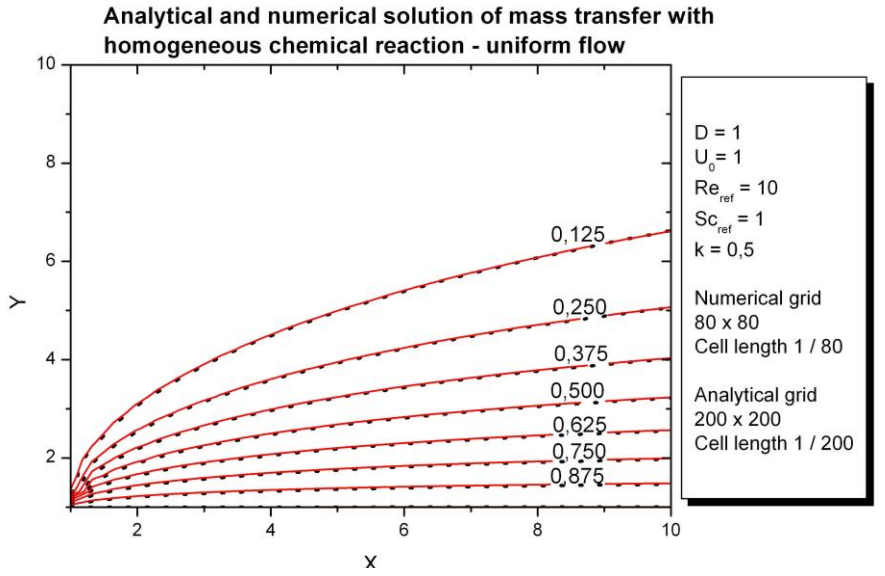


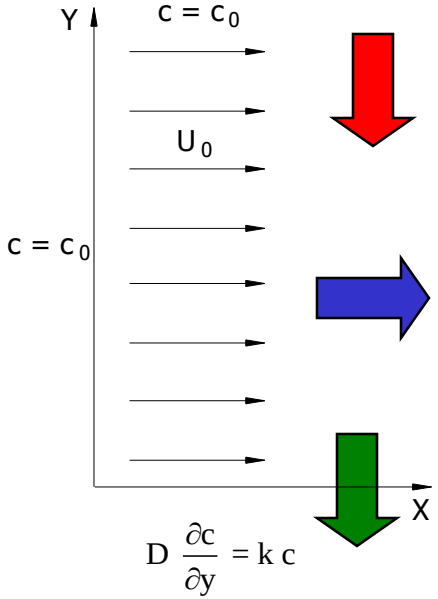
Homogeneous CR

Convection

Diffusion

k = 0.5



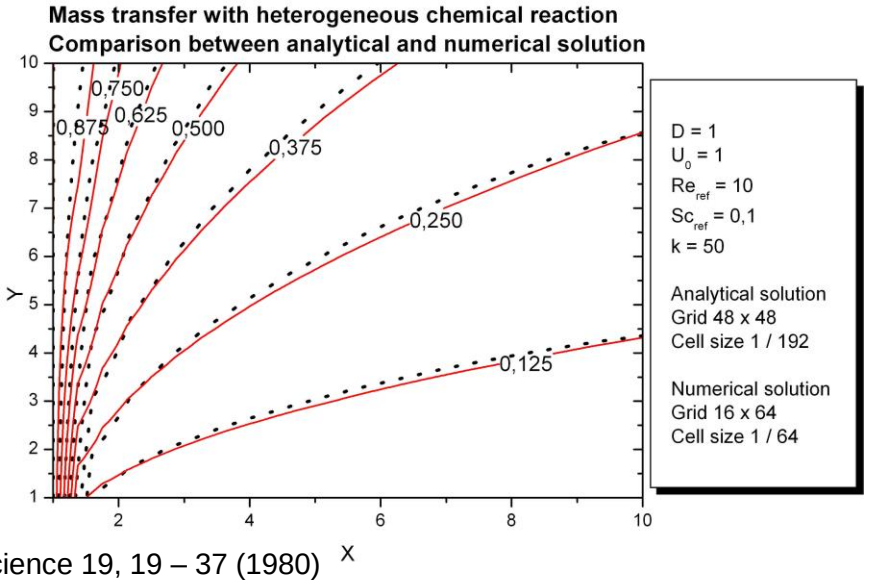


Diffusion

Convection

k = 50

Heterogeneous CR



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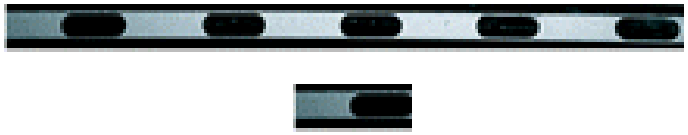
Influence of unit cell length L_{UC} on hydrodynamics

	L_{UC} [mm]	Grid	U_B [m/s]	U_L [m/s]	a [1/m]
A	2.00	48x48x48	0.0964	0.0319	1168.8
B	2.75	48x66x48	0.0964	0.0345	1476.4
C	3.50	48x84x48	0.0969	0.0349	1770.6



H = 0.03

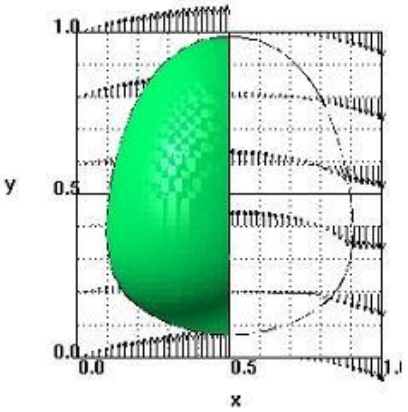
$D_G = 62.24 \times 10^{-6}$ m^2 / s

$D_L = 19.16 \times 10^{-6}$ m^2 / s

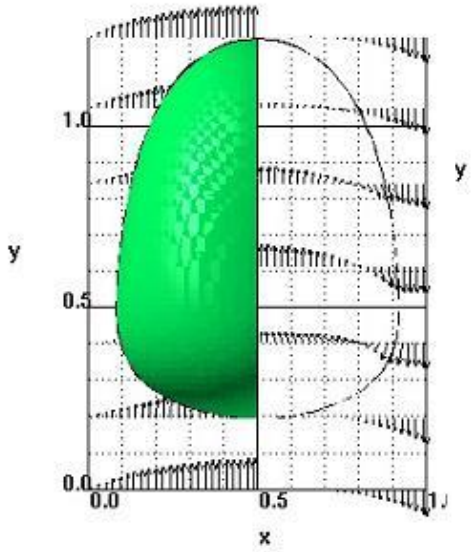
$k^{Het\ CR} = 1500$ s^{-1} $\quad Re_B \sim 10$

$k^{Hom\ CR} = 50$ m / s $\quad Sc \sim 0.8$

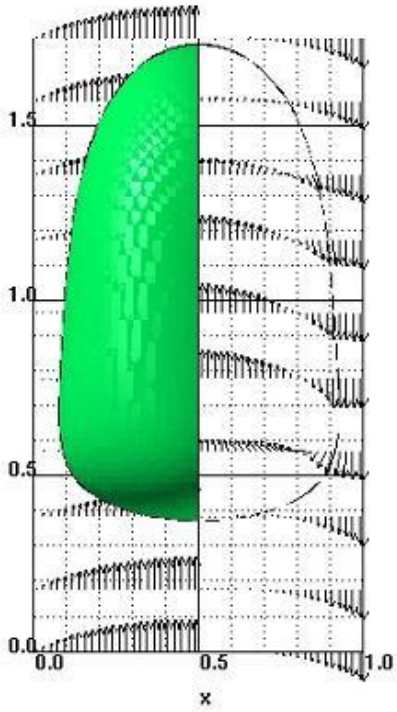
A



B



C



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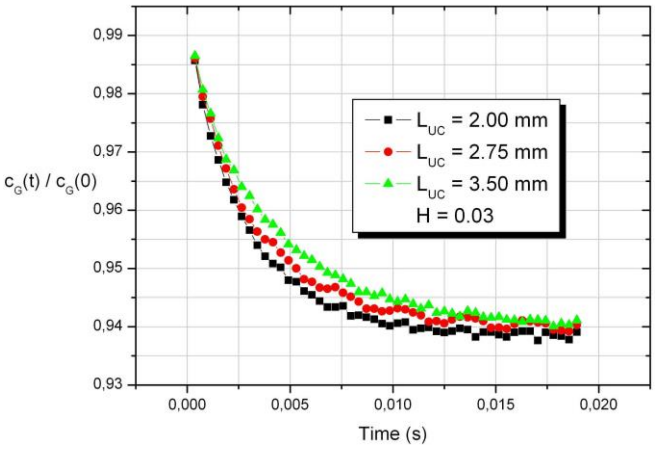
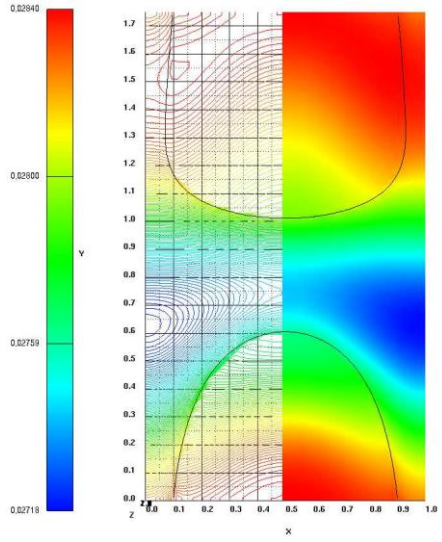
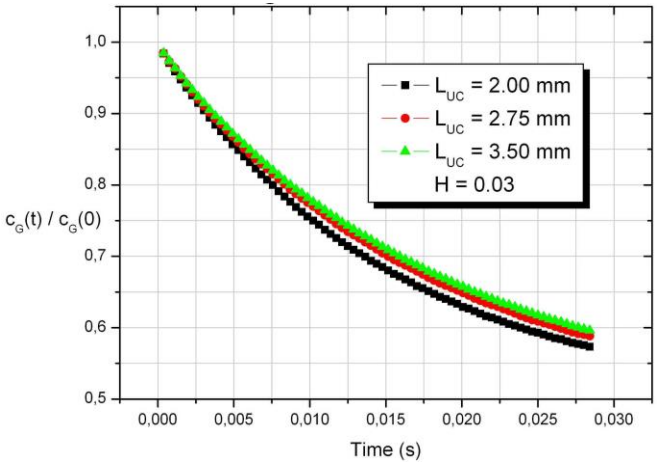
Influence of L_{UC} on mass transfer with and without chemical reaction

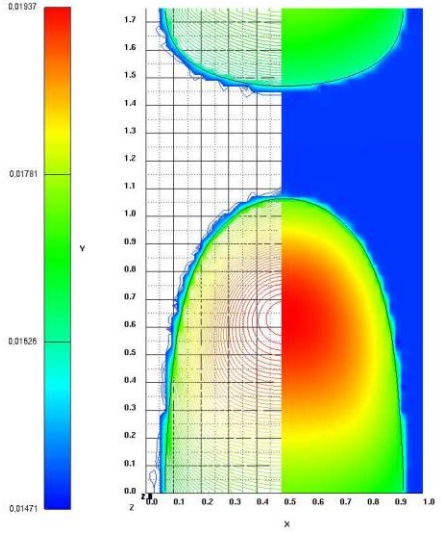
No chemical reaction



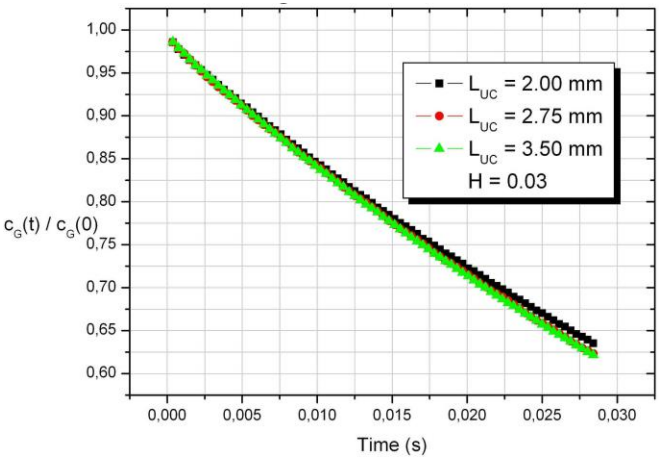


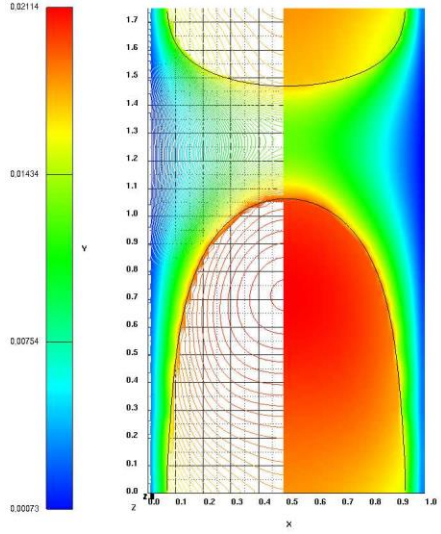
Homogeneous reaction





Heterogeneous reaction





Conclusions

- Implementation of the diffusive term has been successfully validated against 1D and 2D analytical solutions
- Implementation of the source term has been successfully validated against analytical solutions of mass transfer with homogeneous and heterogeneous chemical reaction in single phase flows
- Short unit cells are found more efficient than long unit cells for pure mass transfer and mass transfer accompanied by homogeneous chemical reaction, while long unit cells tend to be more efficient for mass transfer with chemical reaction at the wall

Further step

Numerical simulation of U(VI) transfer from HNO_3 solutions into TBP solution