TWO-PHASE FLOW AND MULTIPHYSICS SIMULATIONS IN COMSOL

By

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Objective and Outline of the Presentation

Objective

- *Share some of the research works carried out at Chemical Engineering Division, BARC using COMSOL Multiphysics*
- *Highlight the capability of COMSOL Multiphysics to simulate problems involving two-phase flow and multiple physics*

Part-1: Two-phase Flow Simulations

- *Drop formation at a single hole in a sieve plate*
- *Air pulsed liquid columns*
- *Liquid-liquid two-phase flow at microfluidic junctions*

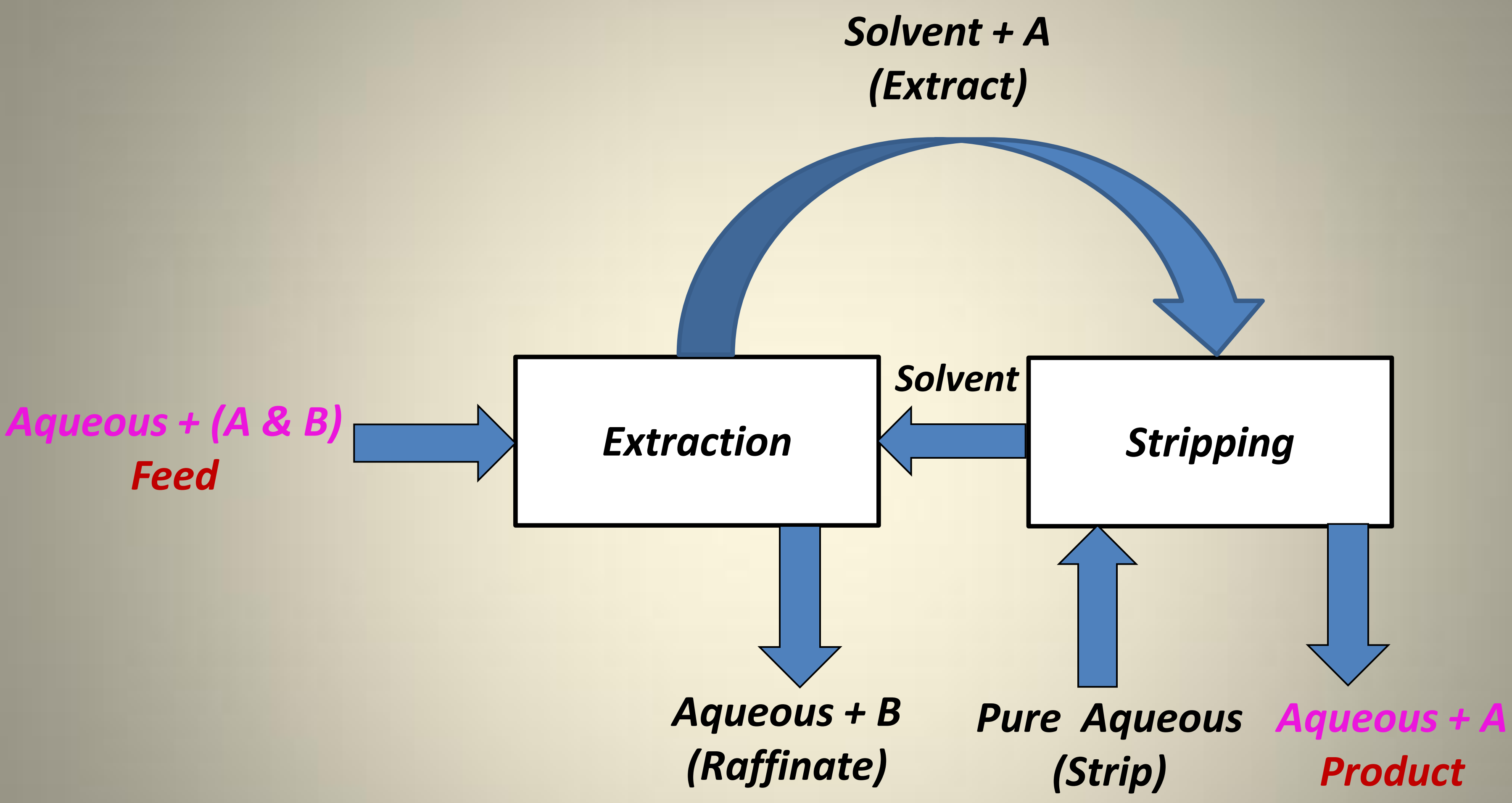
Part-2: Multiphysics Simulations

- *Flow electrolysers*
- *Pore of a supported liquid membrane*
- *Mass transfer for a single droplet*

Part-1

Two-phase Flow Simulations

Drop Formation at a Single Hole



A typical solvent extraction flow sheet

Drop Formation at a Single Hole

- ***Conventional Contactors***
  - *Mixer settlers*
  - *Pulsed columns*
  - *Rotating disk contactors*
  - *Centrifugal extractor*
- ***Novel Contactors***
  - *Microfluidic devices*
  - *Hollow fibre modules*

$$m = K_L a \tau \Delta C$$

$$a = \frac{6\phi}{d_{32}}$$

$m \Rightarrow$ *amount of mass transferred (mol)*

$a \Rightarrow$ *interfacial area (m^2)*

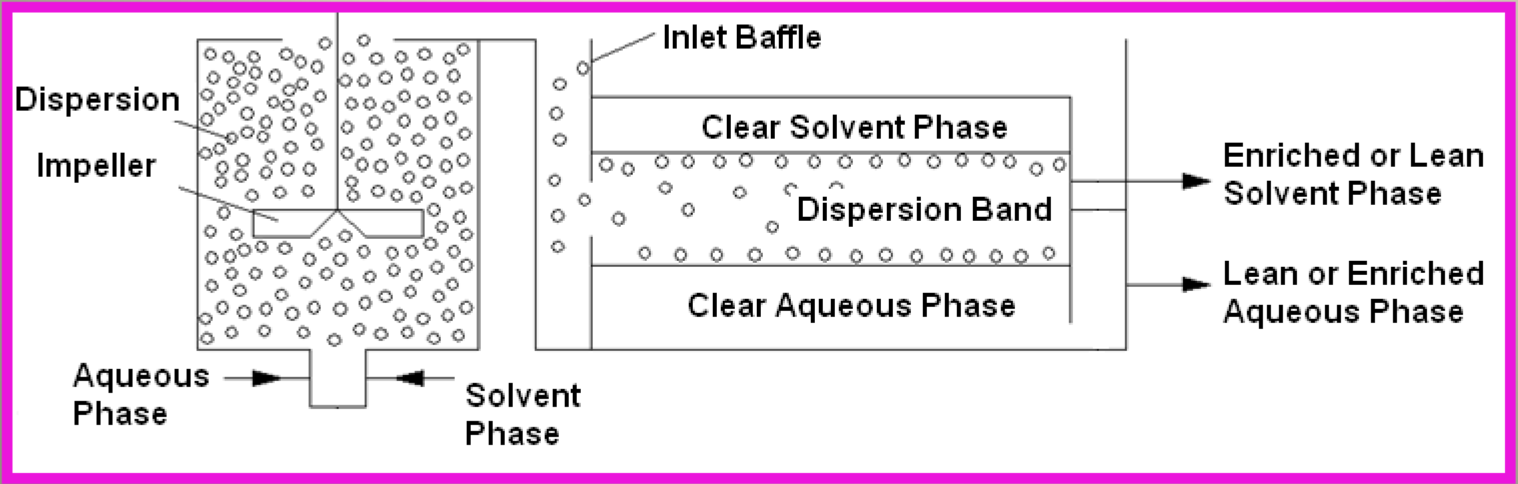
$\tau \Rightarrow$ *contact time (sec)*

$\Delta C \Rightarrow$ *average concentration difference (mol/m^3)*

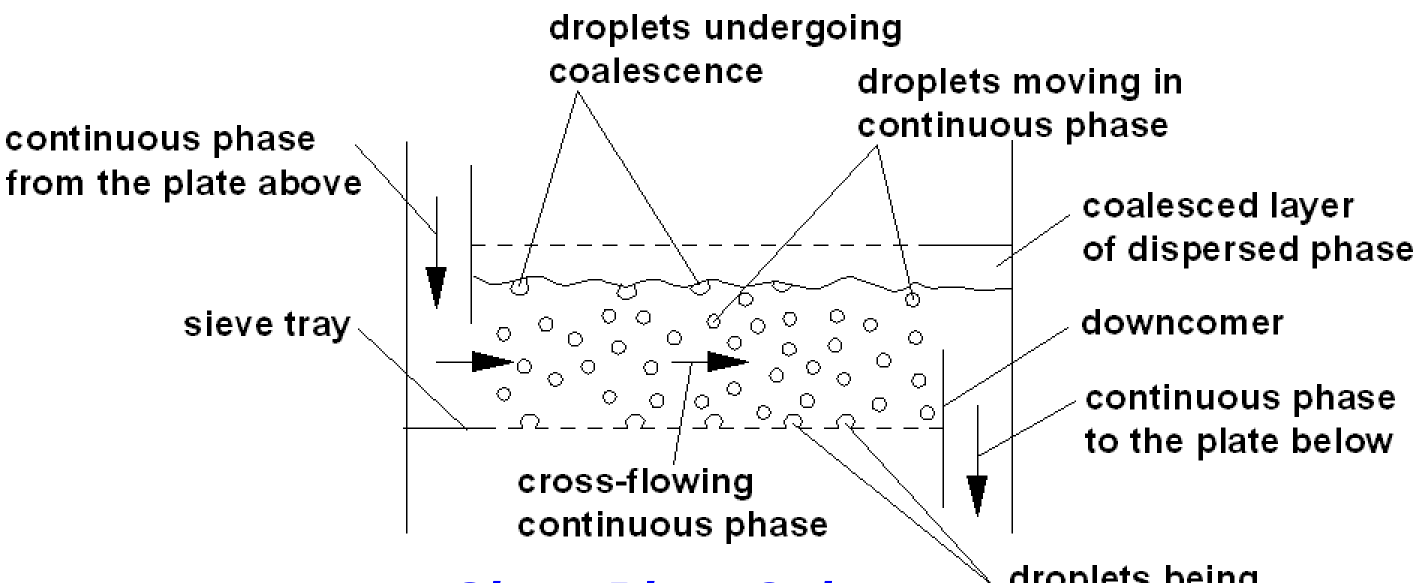
$K_L \Rightarrow$ *mass transfer coefficient (m/s)*

$\phi \Rightarrow$ *volume fraction of dispersed phase (-)*

$d_{32} \Rightarrow$ *Sauter mean diameter (m)*



Drop Formation at a Single Hole

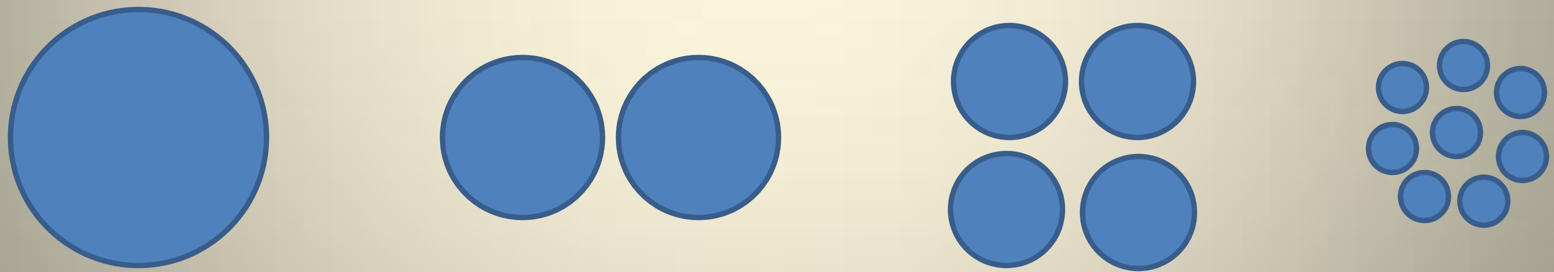


Sieve Plate Column

$$m = K_L a \tau \Delta C$$

$$a = \frac{6\phi}{d_{32}}$$

Drops of an optimum size are required

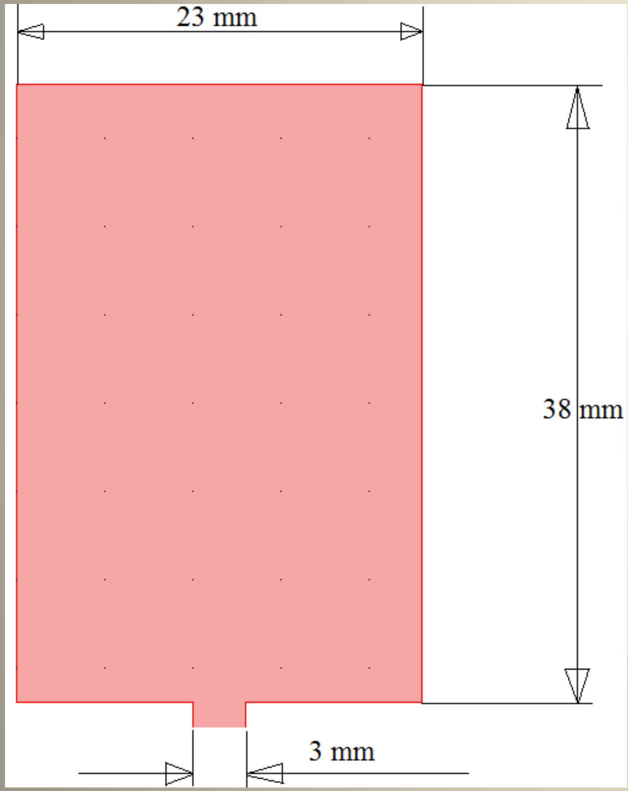


Drop size and hence specific interfacial area will depend on

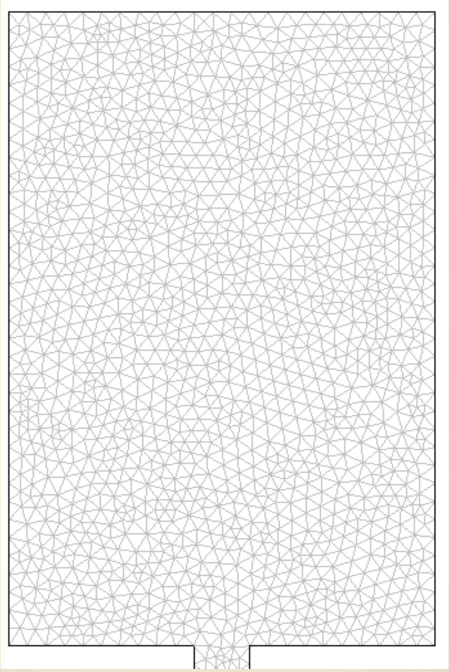
- ***Flow rates***
- ***Physical properties of the continuous and the dispersed phases***
- ***Plate geometry (hole size, type of hole, open area)***

Drop Formation at a Single Hole

- ***Objective was to understand the process of drop formation***
- ***Only one hole was considered***
- ***Continuous phase was considered quiescent***



Computational domain



Meshed computational Domain

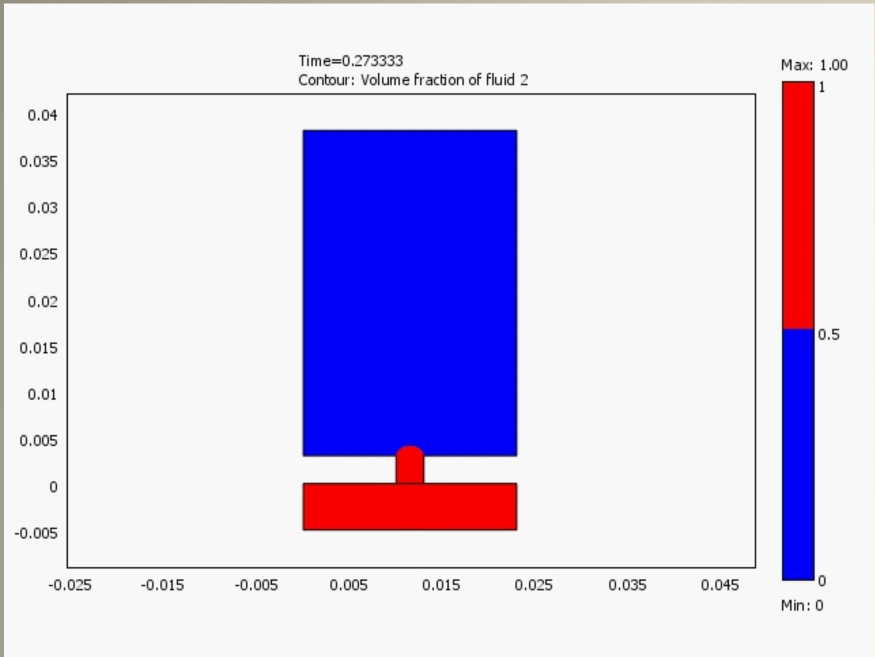
Phase field method for interface tracking

Continuous phase: Water

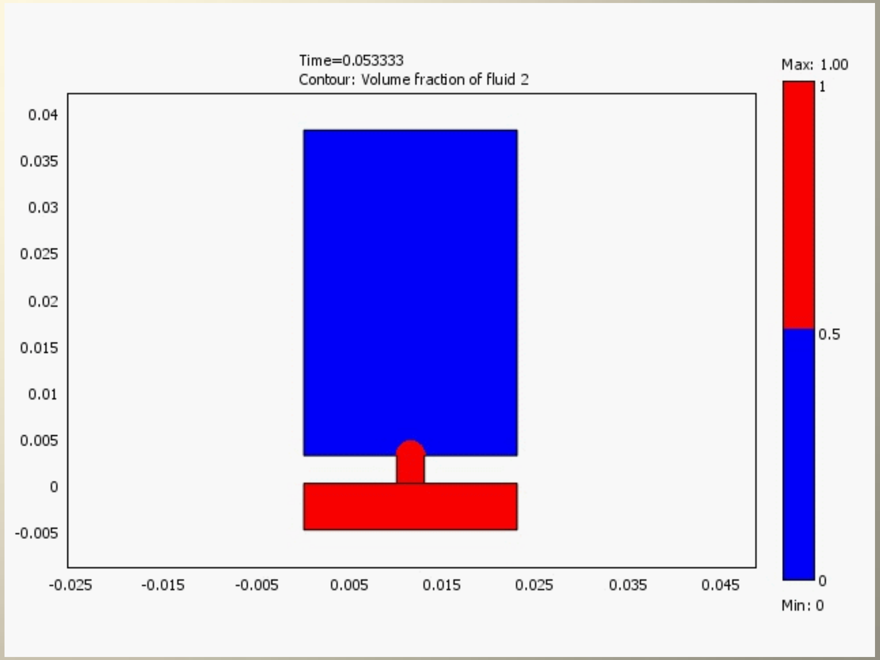
Dispersed phase: Exxol D80

Sen et al., Numerical simulation of drop formation at a hole in quiescent continuous phase, *Accepted in* ***International Congress on Computational Mechanics and Simulations, Hyderabad, 10-12 December, 2012.***

Drop Formation at a Single Hole

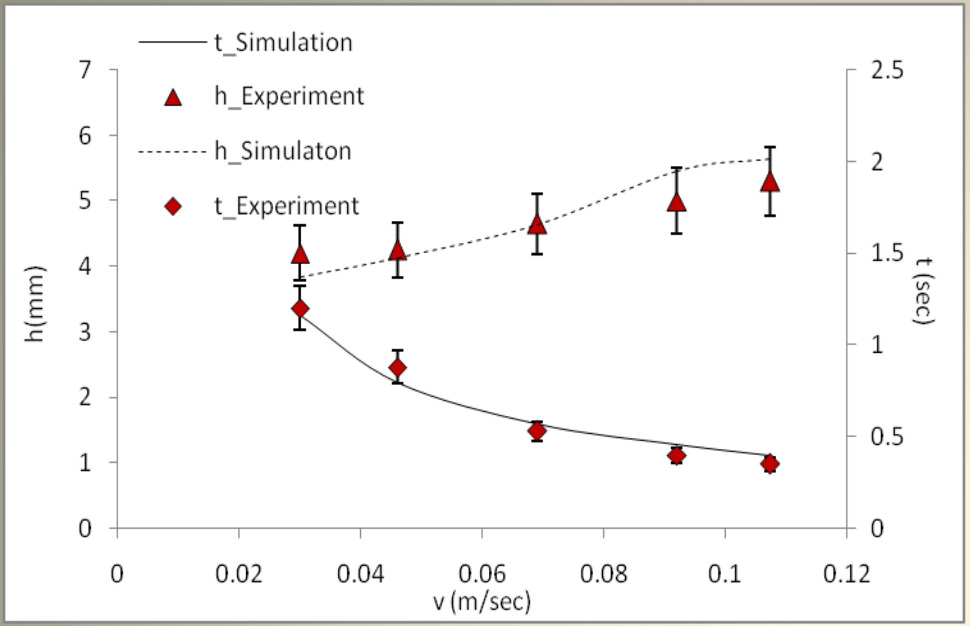


V = 0.03 m/s



V = 0.11 m/s

Drop Formation at a Single Hole



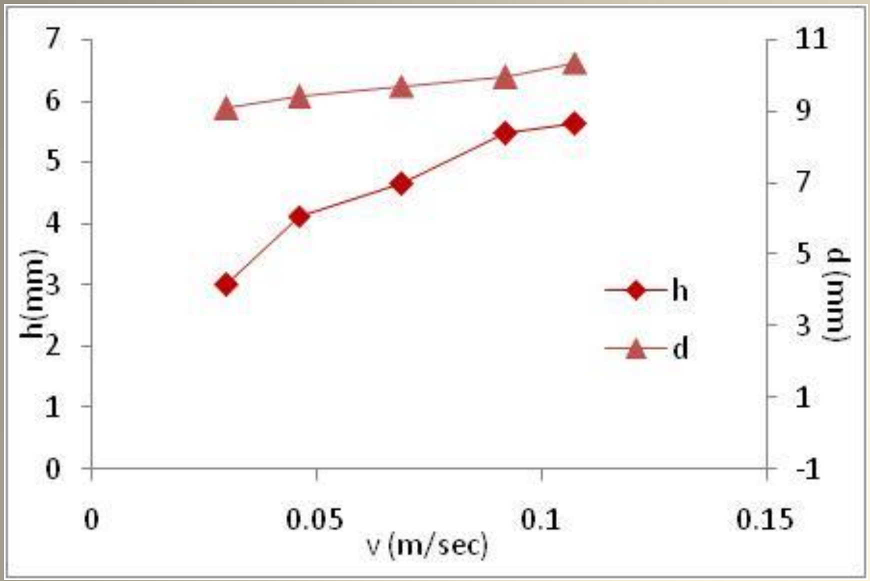
Validation was done using the data reported in literature

Parametric studies were done to understand the effects of following variables on drop formation process

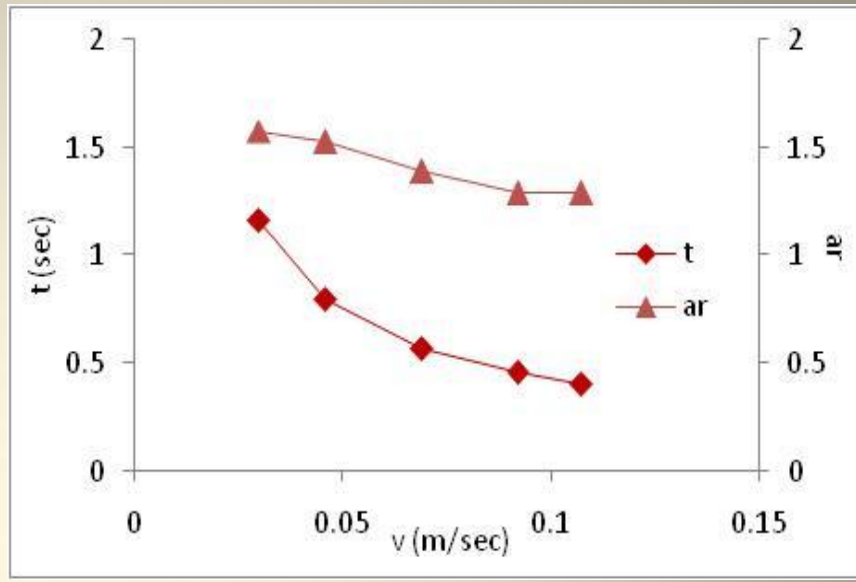
- ***Flow rate***
- ***Physical properties (density, viscosity, interfacial tension, contact angle)***
- ***Geometry (hole diameter, type of hole)***

Soleymani et al., Simulation of drop formation in a single hole in solvent extraction using the volume-of-fluid method, Chem. Eng. Res. Des., 86 (2008), 731-738

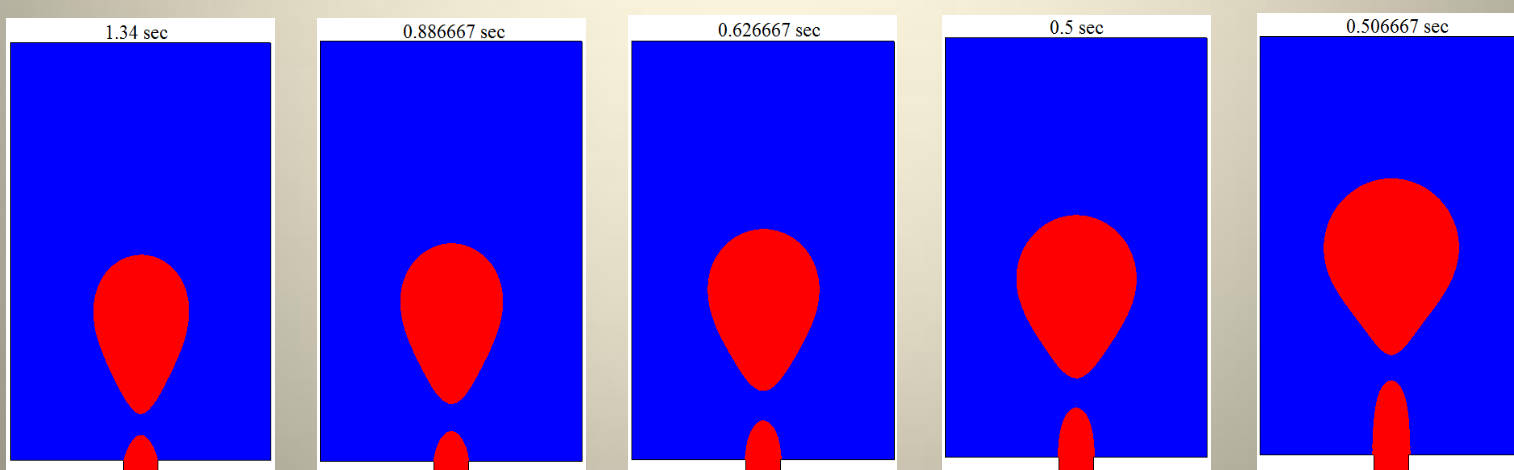
Drop Formation at a Single Hole



Effect of velocity on height of drop detachment and drop diameter



Effect of velocity on time of drop detachment and aspect ratio



0.03 m/sec **0.046 m/sec** **0.069 m/sec** **0.092 m/sec** **0.107 m/sec**

Drop Formation at a Single Hole

$$\frac{dEo^{0.42}}{d_h} = 1.962 - \frac{0.0087487}{Fr} + \frac{0.81402}{\theta^2}$$

$$Eo = \frac{(\rho_C - \rho_D) g d_h^{\ 2}}{\sigma}$$

$$Fr = \frac{v^2}{g d_h}$$

Results from parametric studies were used to obtain a correlation for equivalent drop diameter

d $\Rightarrow$ ***Equivalent drop diameter (m)***

d_h $\Rightarrow$ ***Hole diameter (m)***

θ $\Rightarrow$ ***Contact angle (radian)***

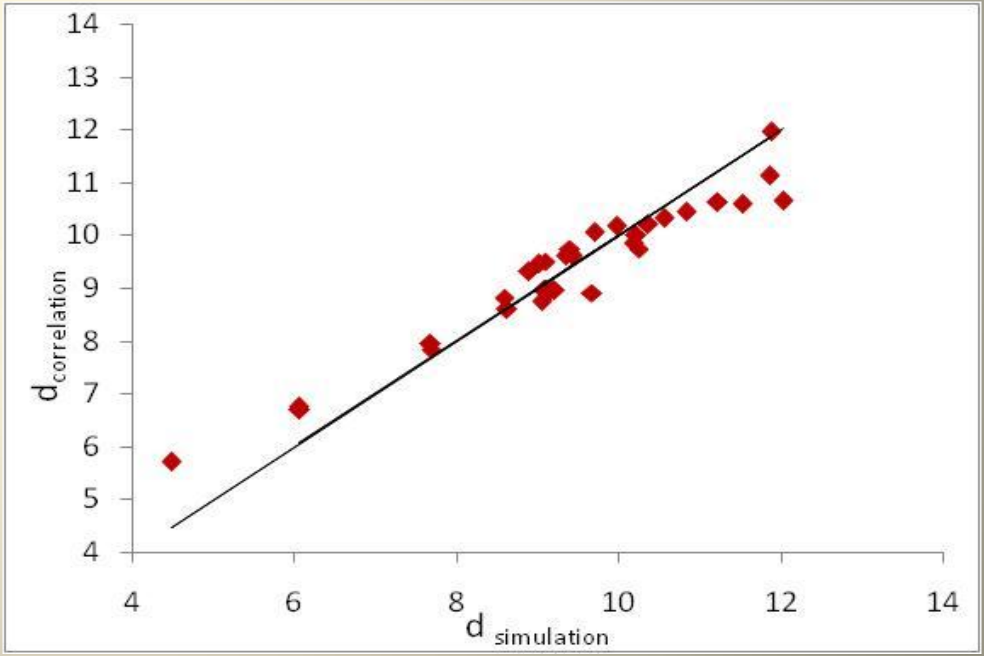
Eo $\Rightarrow$ ***Eotvos number***

Fr $\Rightarrow$ ***Froude number***

ρ_C $\Rightarrow$ ***Density of the continuous phase***

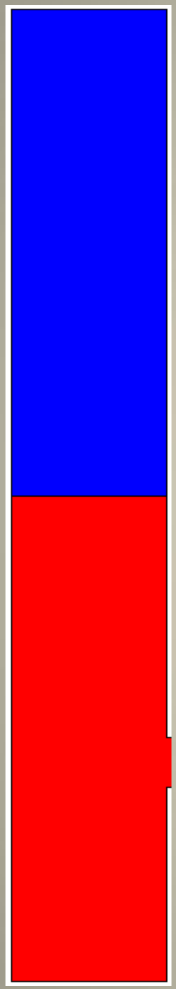
ρ_D $\Rightarrow$ ***Density of the dispersed phase***

σ $\Rightarrow$ ***Interfacial tension***

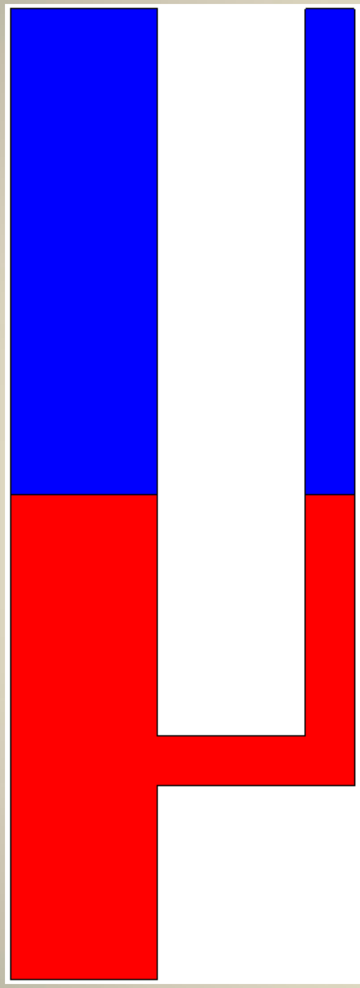


The study helps us understand the process of drop formation at a single hole

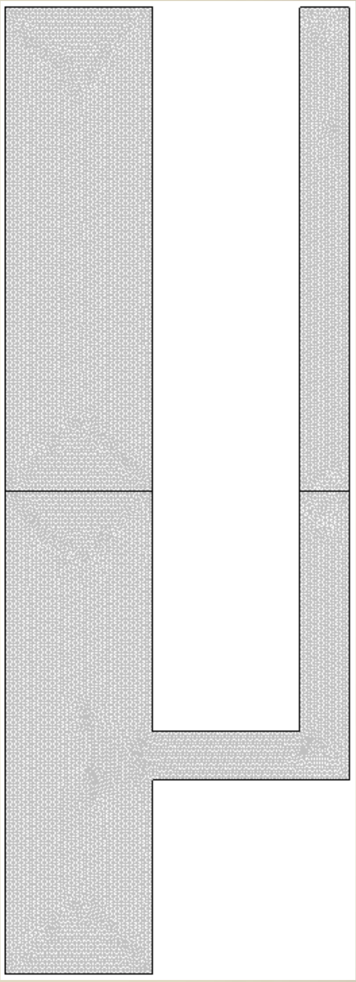
Air Pulsed Liquid Column



Liquid column



Liquid column with pulse leg



Meshed computational domain

Column height 1 m
Column diameter 6 inch
Pulse leg size 2 inch

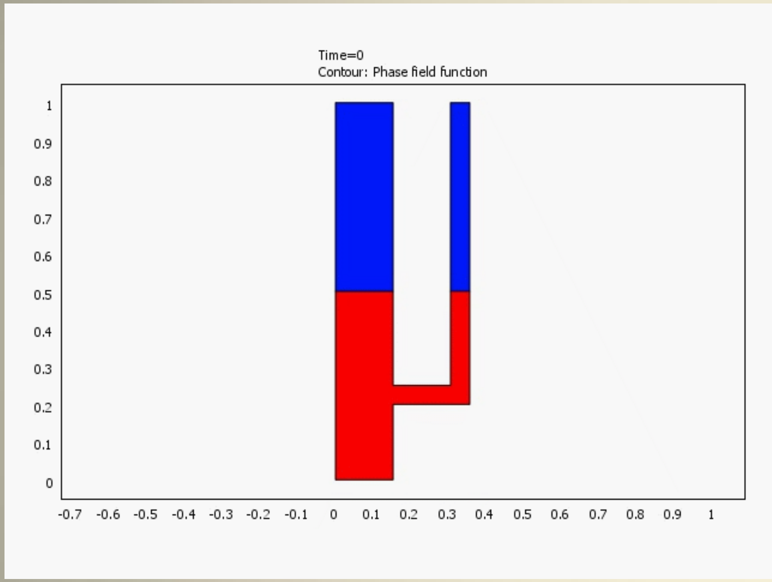
Phase field method was used for interface tracking

Laminar flow of water and air

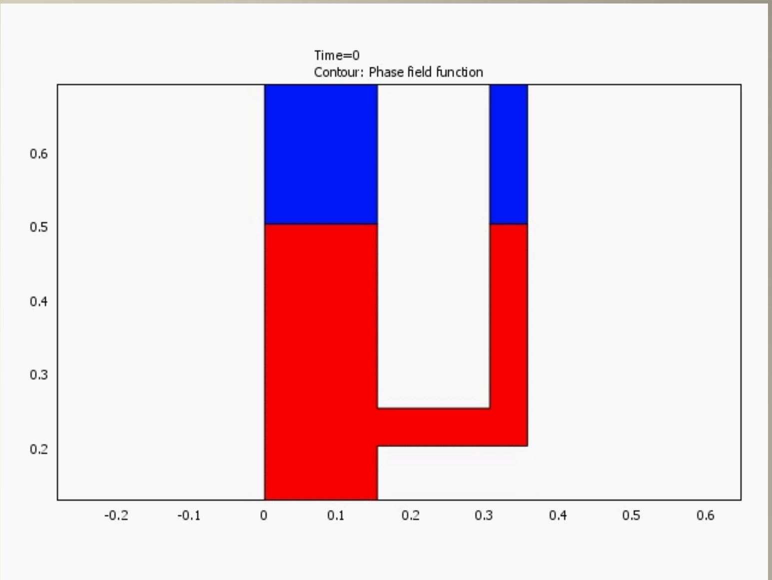
Cyclic air pressure applied at pulse leg

2D simulations

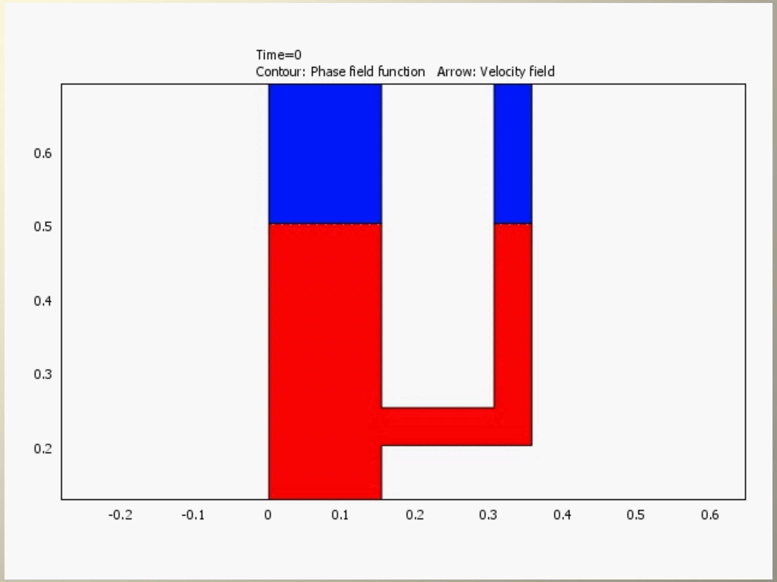
Air Pulsed Liquid Column



Animation showing movement of liquid level in the column and pulse leg

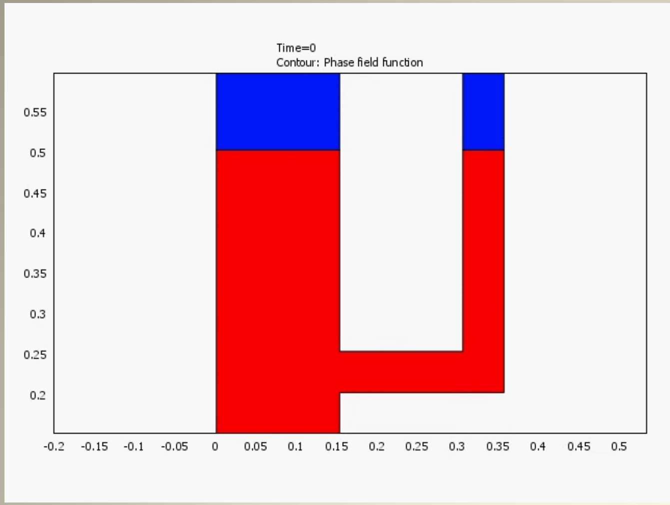


Closer look at the interfaces

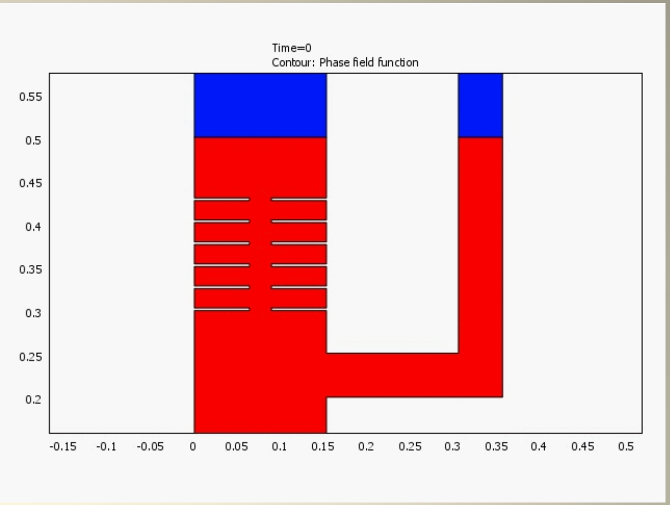


Velocity Vectors

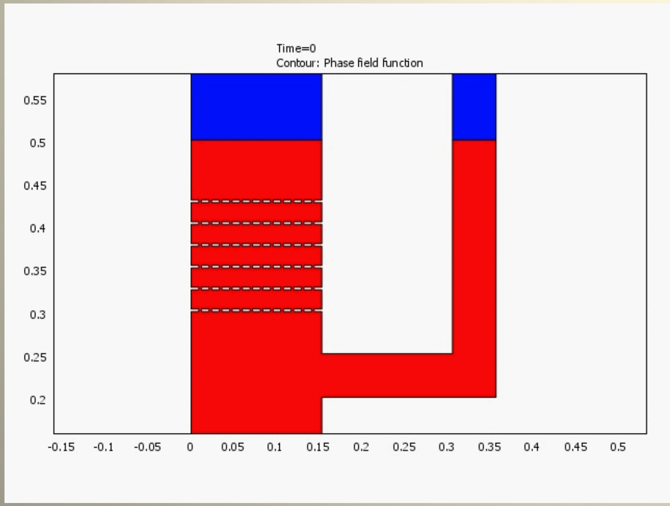
Air Pulsed Liquid Column



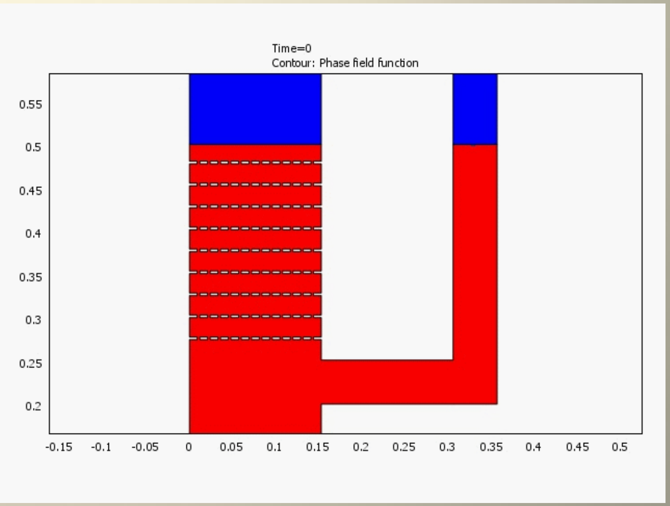
Column without internals



Column with orifice plates

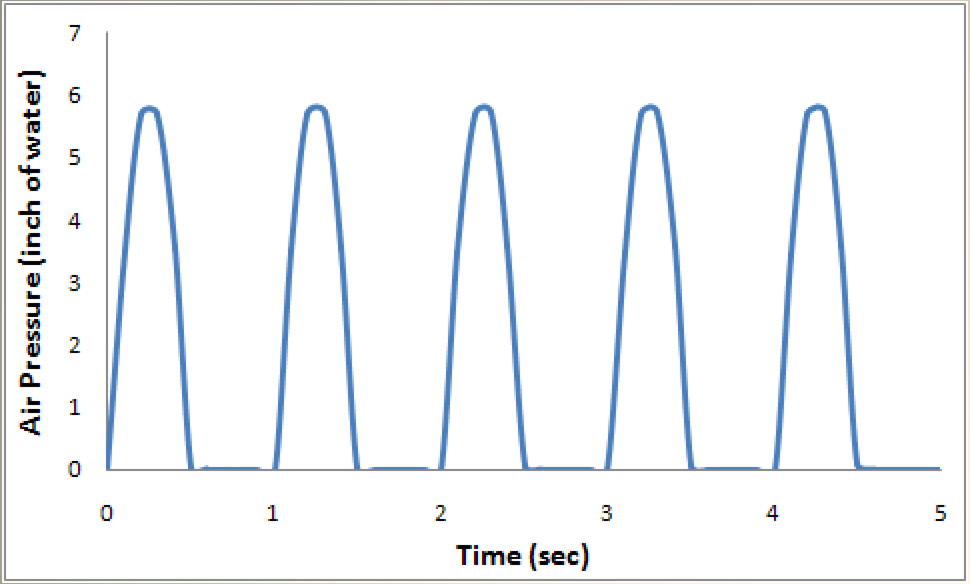


Column with 6 sieve plates



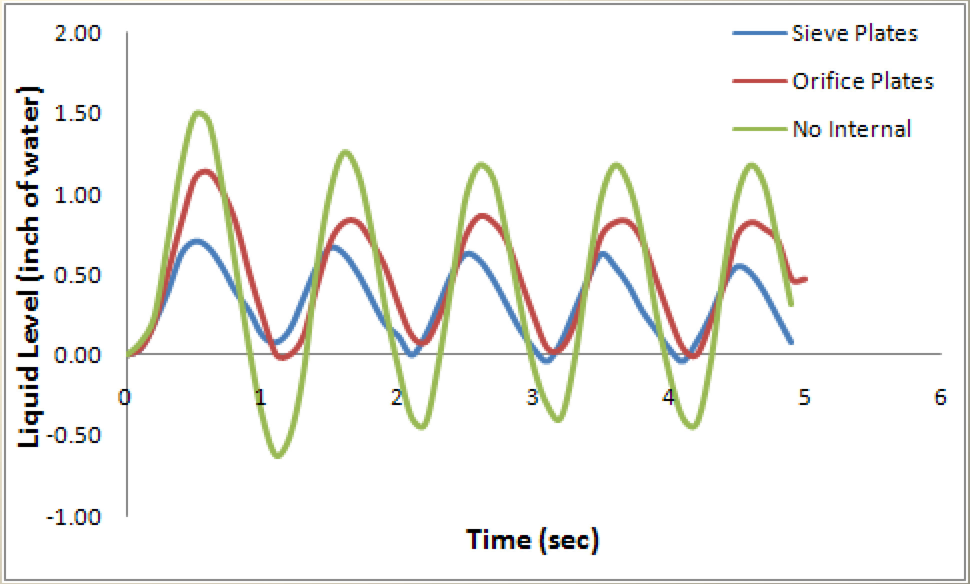
Column with 9 sieve plates

Air Pulsed Liquid Column



Simulations results are as expected i.e. amplitude of liquid level fluctuation for a given air pressure cycle reduces as the pressure drop attributable to the internals in the column increases

The simulations can be used to fix the air pressure cycle for a desired amplitude of liquid level fluctuation in the column.



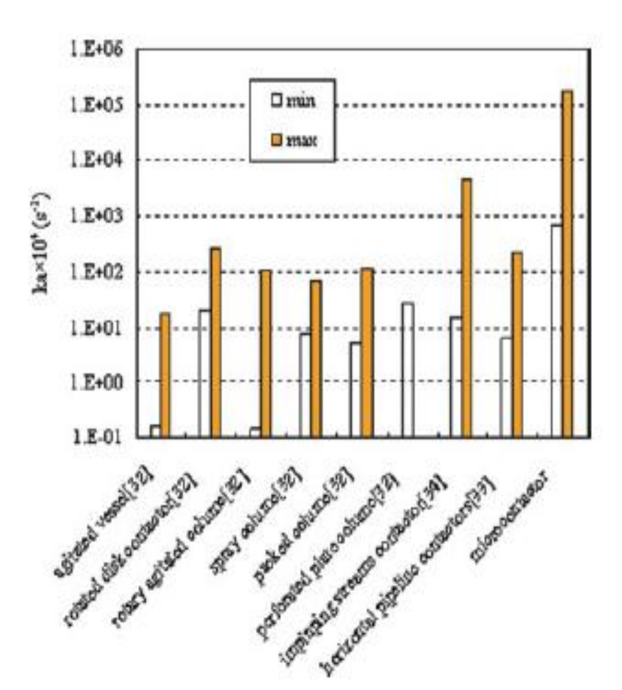
L-L Two-phase Flow at Microfluidic Junctions

Advantages of Microfluidic Devices

- *High specific interfacial area for heat transfer and multiphase applications*
- *Less uncertainty in scale up*
- *Low inventory (better for hazardous chemicals)*
- *Uninterrupted production*
- *In situ production / distributed production*

Advantages of SX in Microchannels

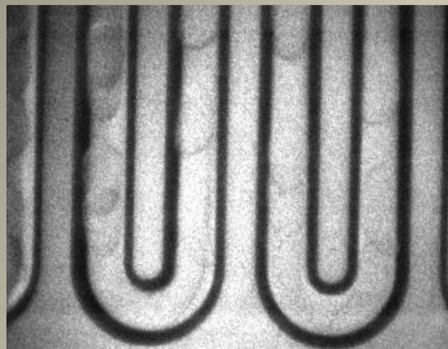
- *High specific interfacial area (low contact time)*
- *Ordered and controllable flow patterns*
- *Monodispersed droplets (ease in phase separation)*



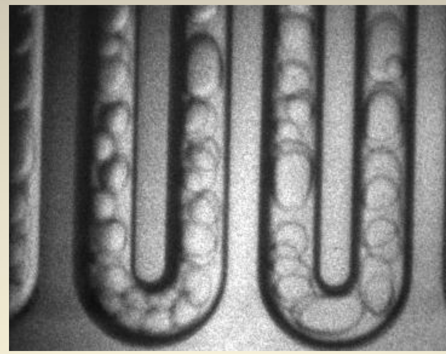
Comparison of overall mass transfer coefficients in different SX equipment

Zhao et al., Liquid-liquid two-phase mass transfer in the T-junction microchannels, AIChEJ, 53 (2007), 3042-3053

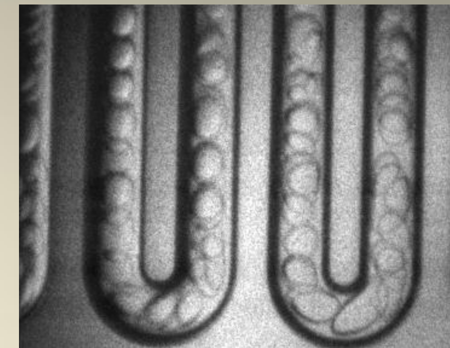
L-L Two-phase Flow at Microfluidic Junctions



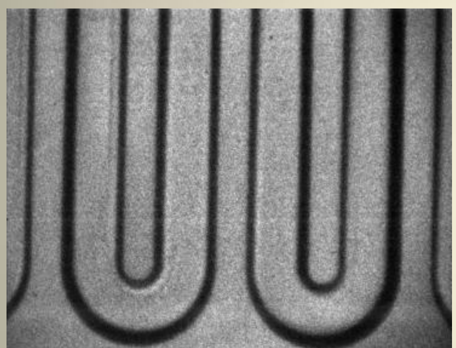
Slug Flow



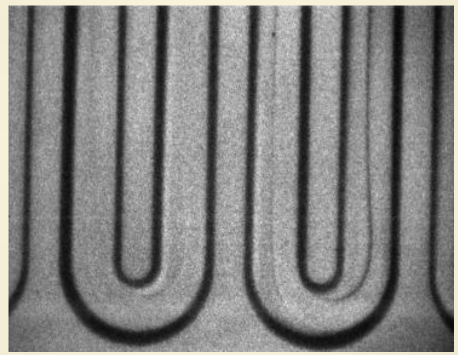
Slug and Droplet Flow



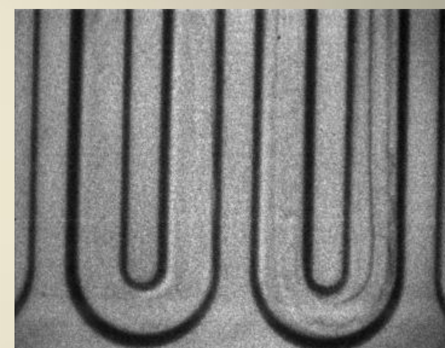
Droplet Flow



Unstable Annular Flow

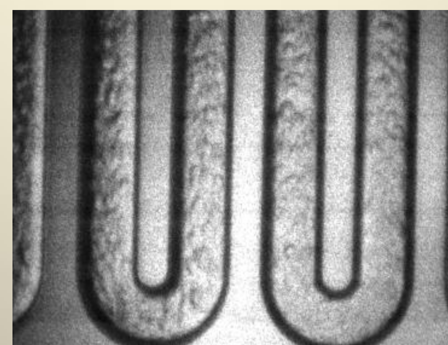


Annular Flow



Annular Dispersed Flow

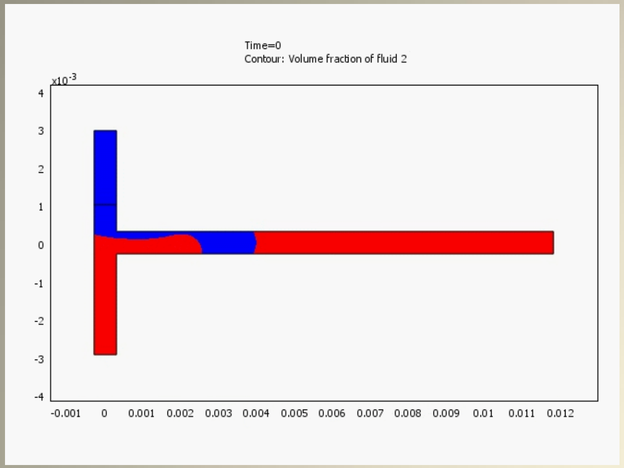
Different types of L-L flow patterns observed in a serpentine microchannel for water butanol system



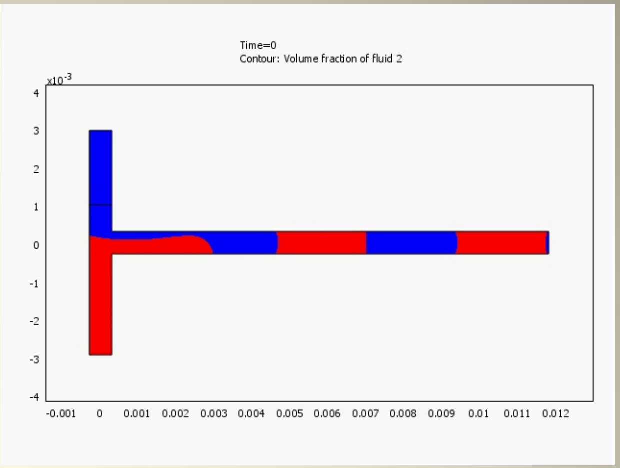
Fully Dispersed Flow

Sarkar et al., Liquid-liquid two-phase flow patterns in a serpentine microchannel, I&ECR, 51 (2012), 5056-5066

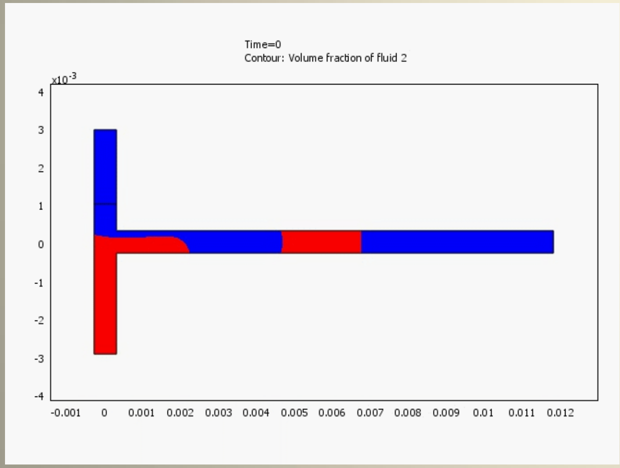
L-L Two-phase Flow at Microfluidic Junctions



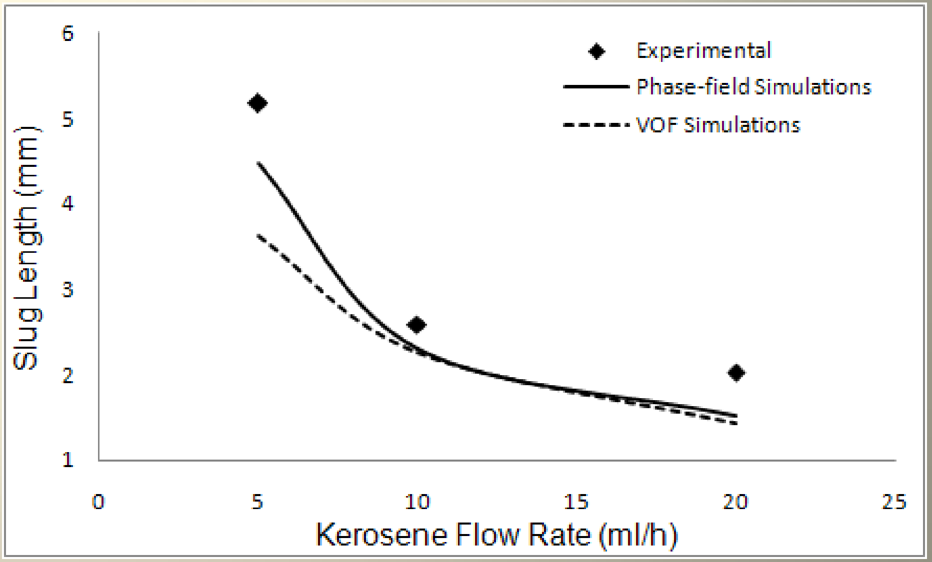
V_d = 0.942 cm/s
V_c = 0.471 cm/s



V_d = 0.942 cm/s
V_c = 0.942 cm/s



V_d = 0.942 cm/s
V_c = 1.883 cm/s

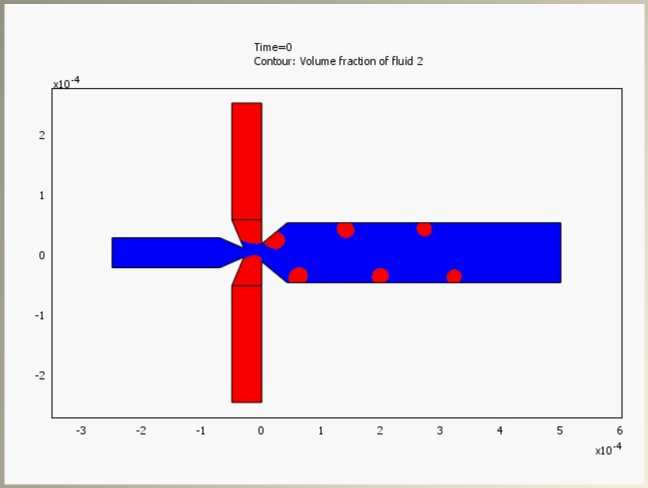


Red Color — ***Kerosene***

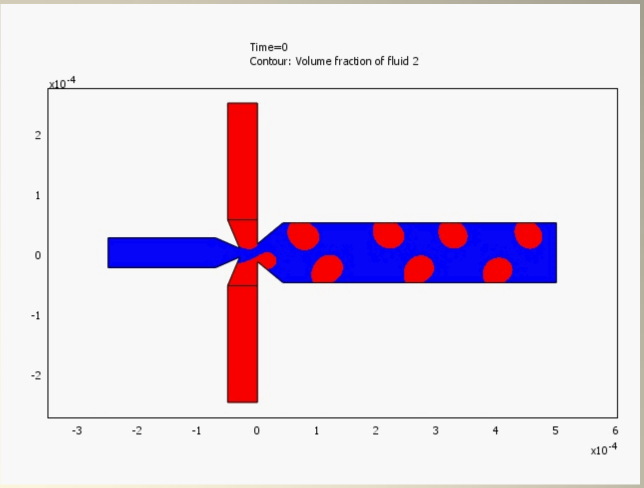
Blue Color — ***Water***

Cherlo et al., Experimental and numerical investigations of two-phase (liquid-liquid) flow behavior in rectangular microchannels, I&ECR, 49 (2010), 893-899

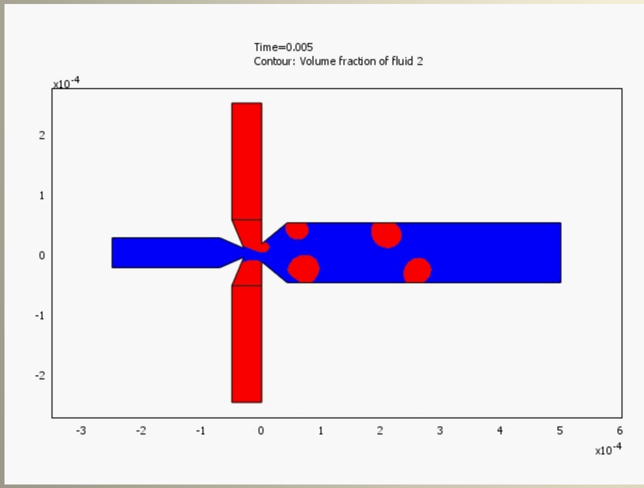
L-L Two-phase Flow at Microfluidic Junctions



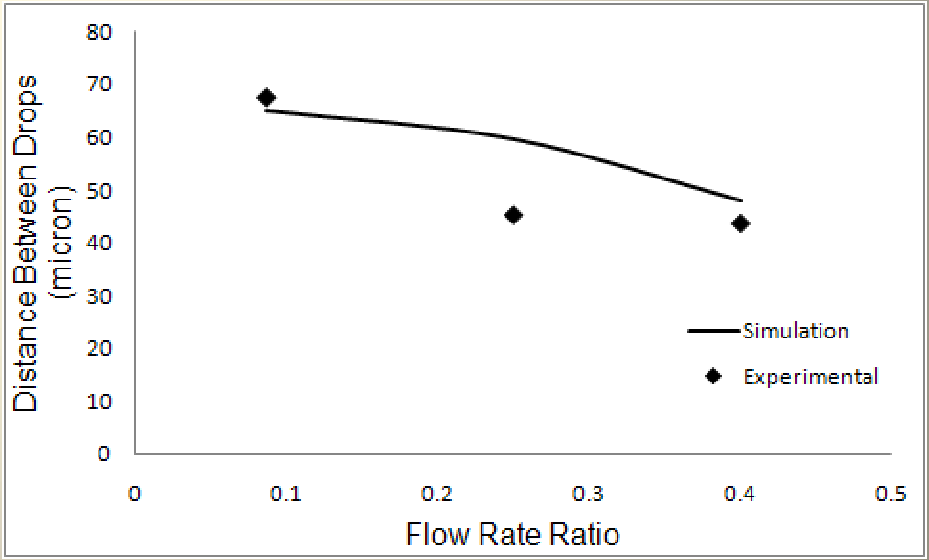
V_d = 0.067 cm/s
V_c = 1.53 cm/s



V_d = 0.167 cm/s
V_c = 1.33 cm/s



V_d = 0.267 cm/s
V_c = 1.33 cm/s

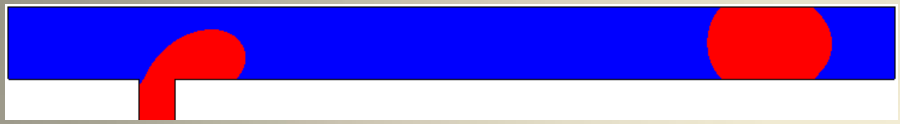


Red Color — ***Water***

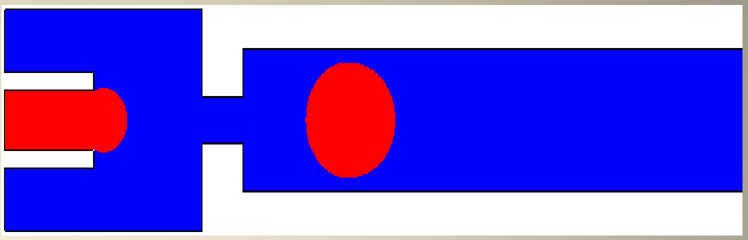
Blue Color — ***Olive Oil***

Mehrotra et al., Monodispersed polygonal water droplets in microchannel. Applied Physics Letters, 92 (2008), 213109.

L-L Two-phase Flow at Microfluidic Junctions



Cross-flow T-junction



Flow Focusing Junction

- ***Numerical simulations can be used to predict liquid-liquid two-phase flow patterns at microfluidic junctions if geometry, flow conditions and physical properties are known***
- ***Numerical simulations can serve as a screening tool to zero in on a geometry that will give the desired flow pattern***

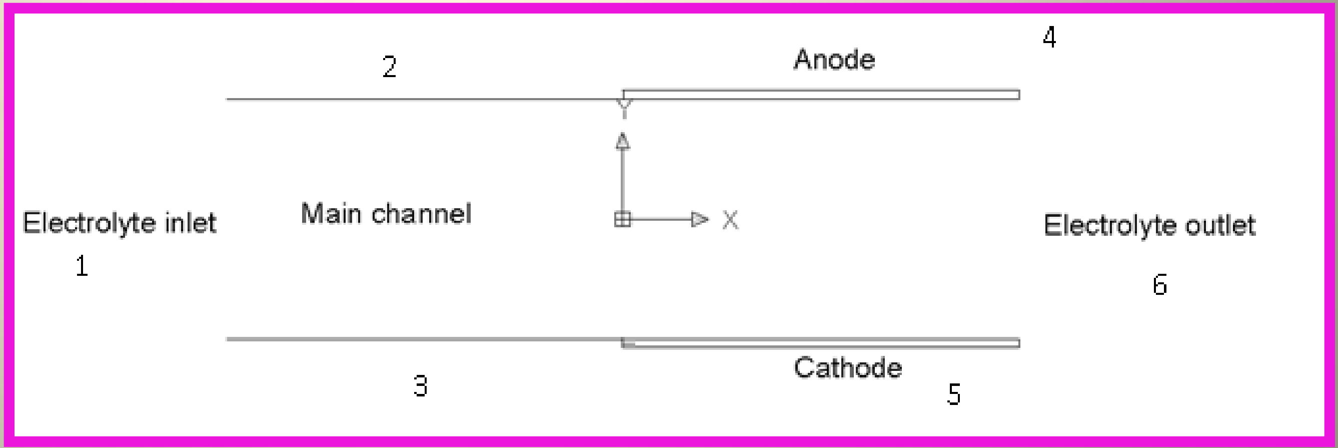
Singh et al., Numerical simulation of liquid-liquid two-phase flow at microfluidic junctions. 3rd European Conference on Microfluidics, Heidelberg, Germany, 3-5 December 2012.

Part-2
Multiphysics Simulations

Numerical Simulation of Flow Electrolysers

- *To study the effect of flow field on the performance of electro-neutral bulk of a flow electrolyzer having stationary cathode*
- *Simulation of flow electrolyser having streaming mercury cathode*
- *Coupled solution of Navier-Stokes and Nernst-Planck equations*
- *Validation of the computational approach was done using the data reported in literature*

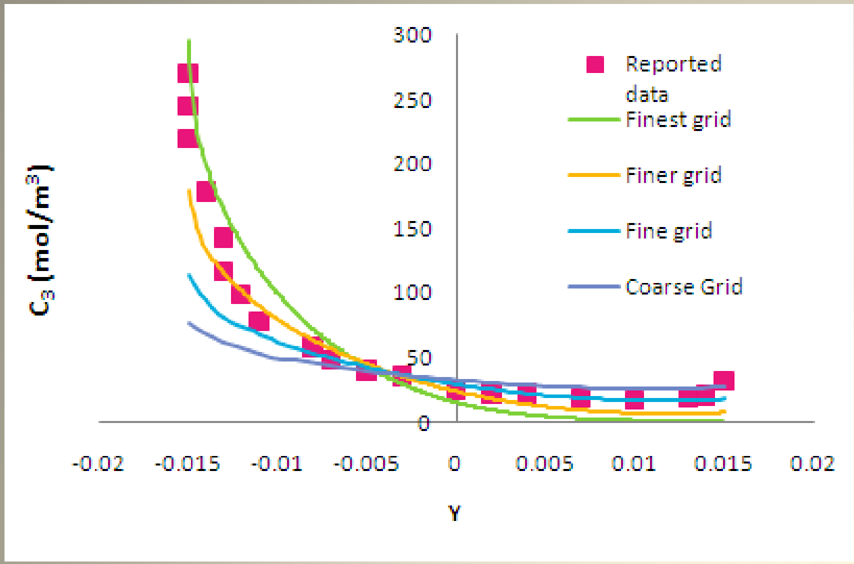
Reactions:
$2Cl^- \rightarrow Cl_2\uparrow + 2e^-$
(at the anode)
$2H_2O + 2e^- \rightarrow 2OH^- + H_2\uparrow$
(at the cathode)
Na^+, Cl^-, OH^- are the ions.



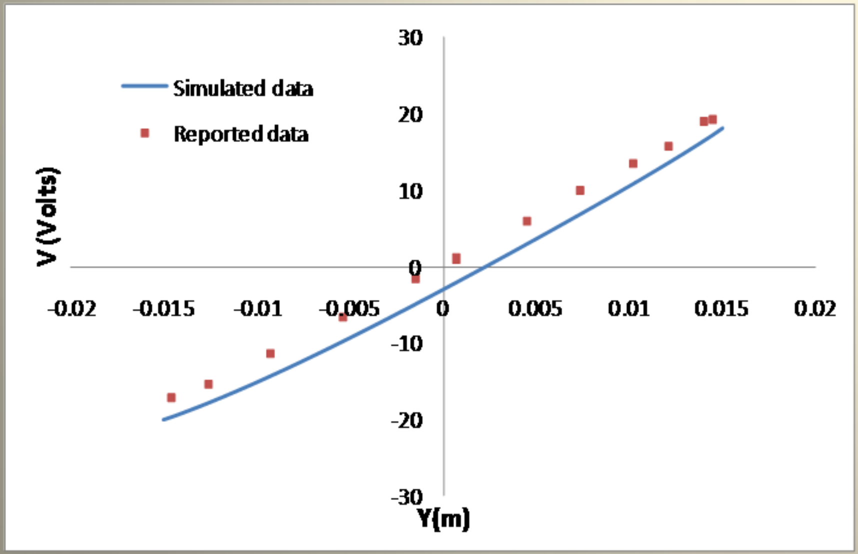
Domain used for validating the computational approach

Lu et al., Numerical simulation of salt water electrolysis in parallel plate electrode channel under forced convection. Electrochimica Acta, 53 (2007), 768-776.

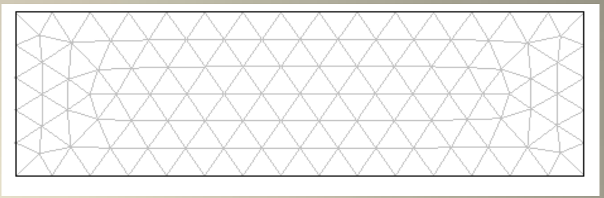
Numerical Simulation of Flow Electrolysers



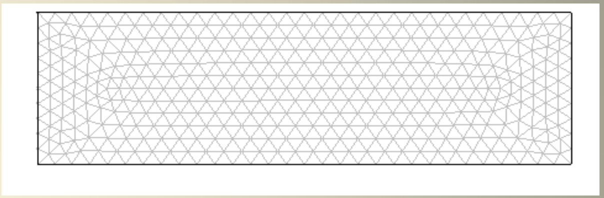
Concentration profile at the outlet



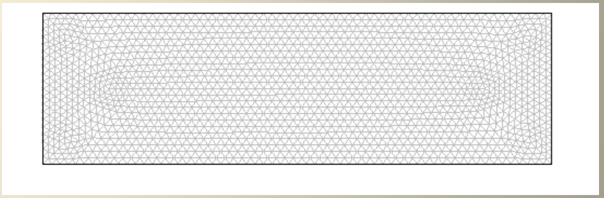
Potential profile at the outlet



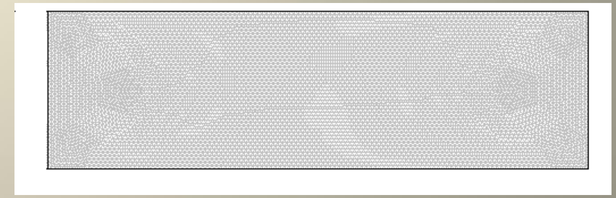
6 elements/cm^2



26 elements/cm^2

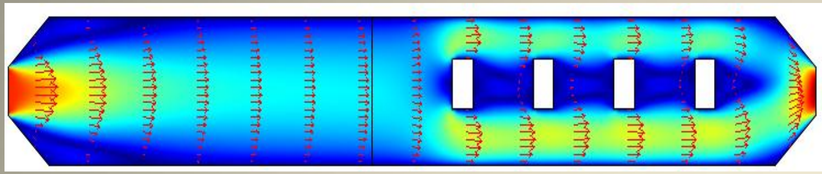


103 elements/cm^2

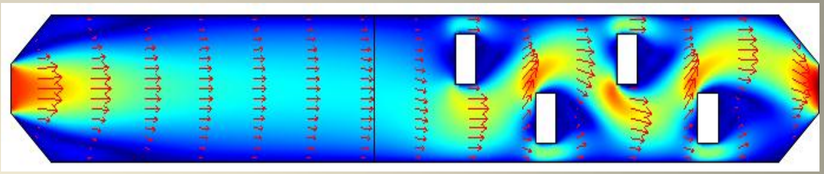


211 elements/cm^2

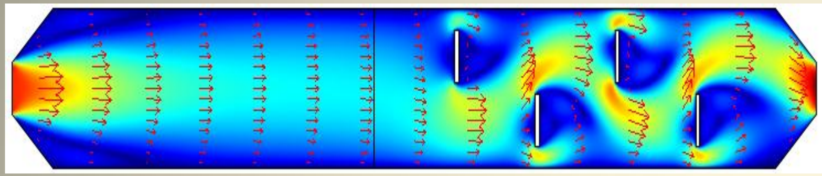
Numerical Simulation of Flow Electrolysers



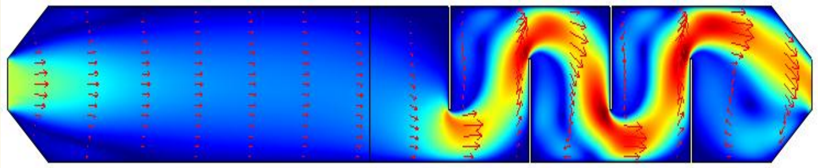
Thick rectangular obstacles



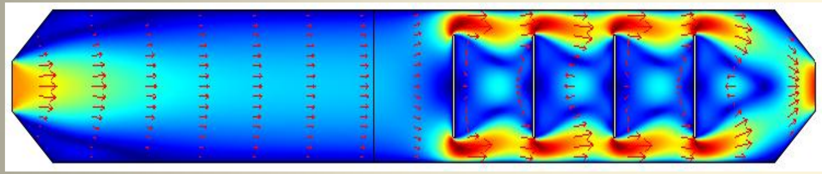
Thick rectangular obstacles



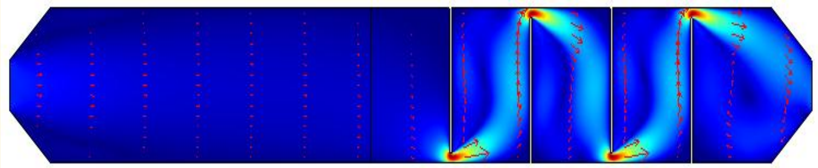
Thin rectangular obstacles



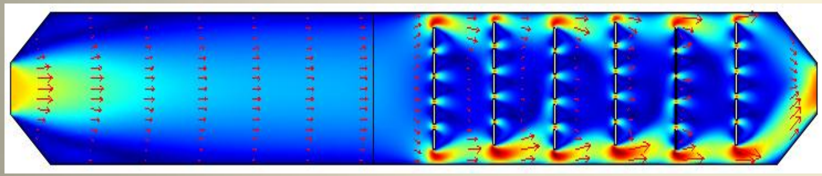
Baffles in flow path



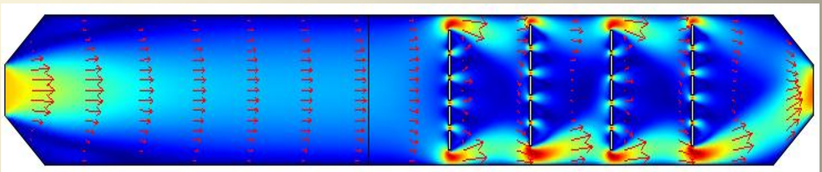
Baffles in flow path



Baffles in flow path



Mesh in flow path



Mesh in flow path

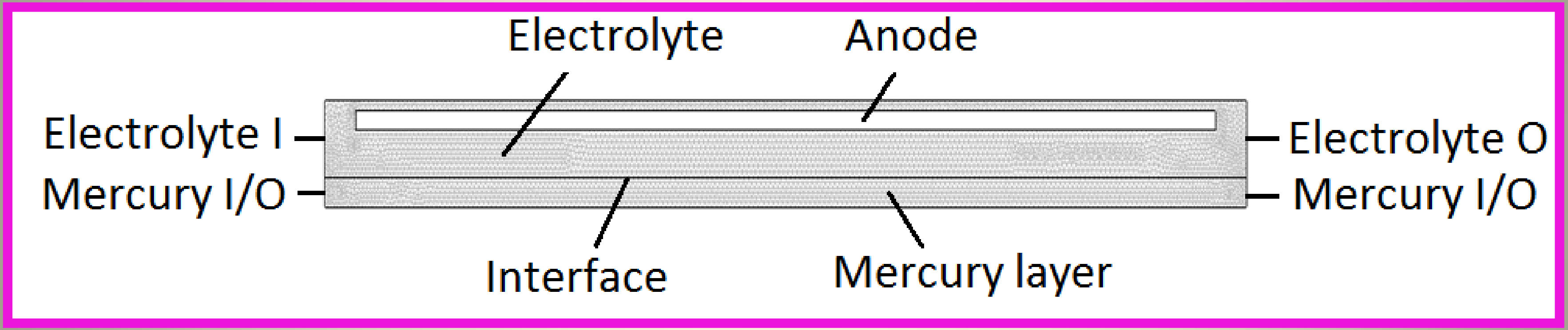
Obstacles ensuring higher velocities close to anode and cathode (mesh type obstacles and baffles in the centre) may lead to better performance of electro-neutral bulk.

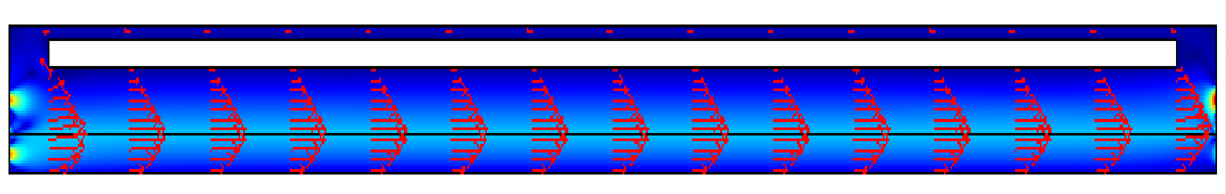
Shukla et al., Numerical simulation of flow electrolysers: effect of obstacles, 79 (2012), 57-66.

Numerical Simulation of Flow Electrolysers

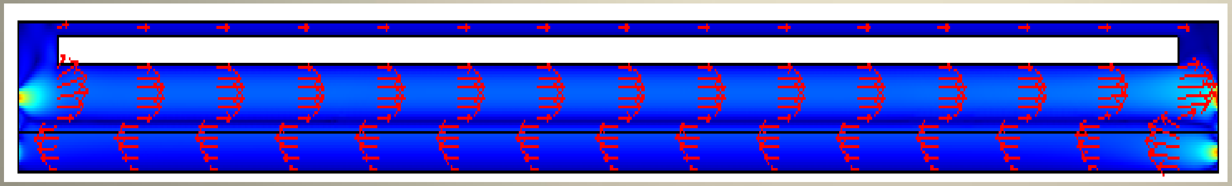
Numerical Simulation of flow electrolyser with streaming mercury cathode

- ***Comparison of co-current and counter-current configurations***
- ***Effect of mercury flow rate***





Current density 62691 (A/m^2)



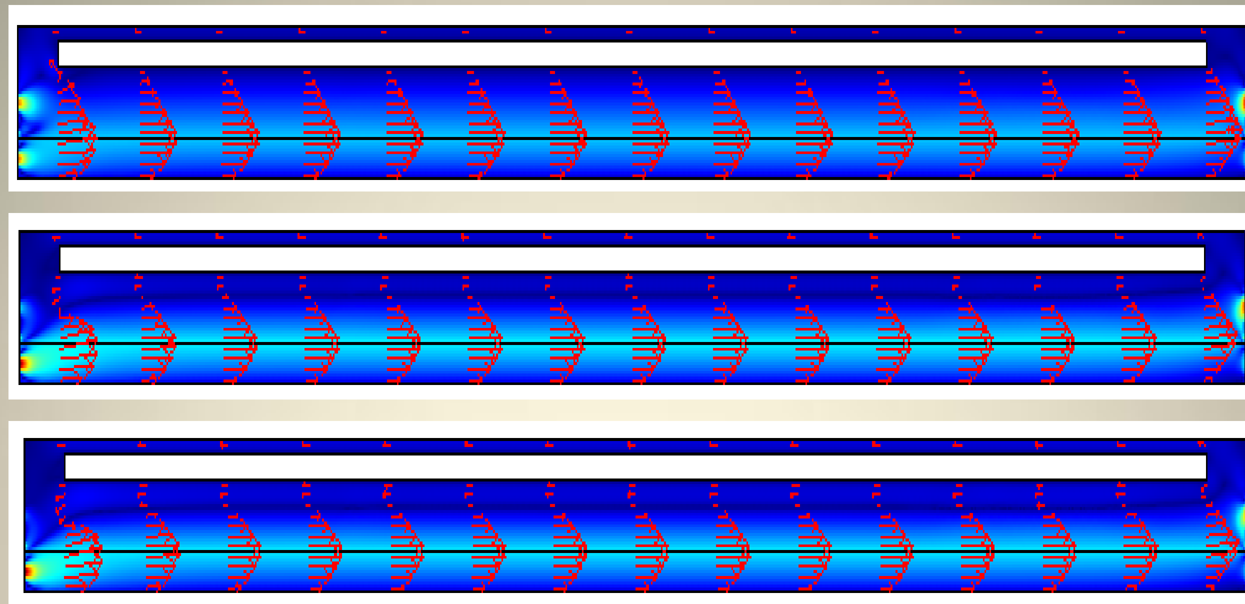
Current density 58785 (A/m^2)

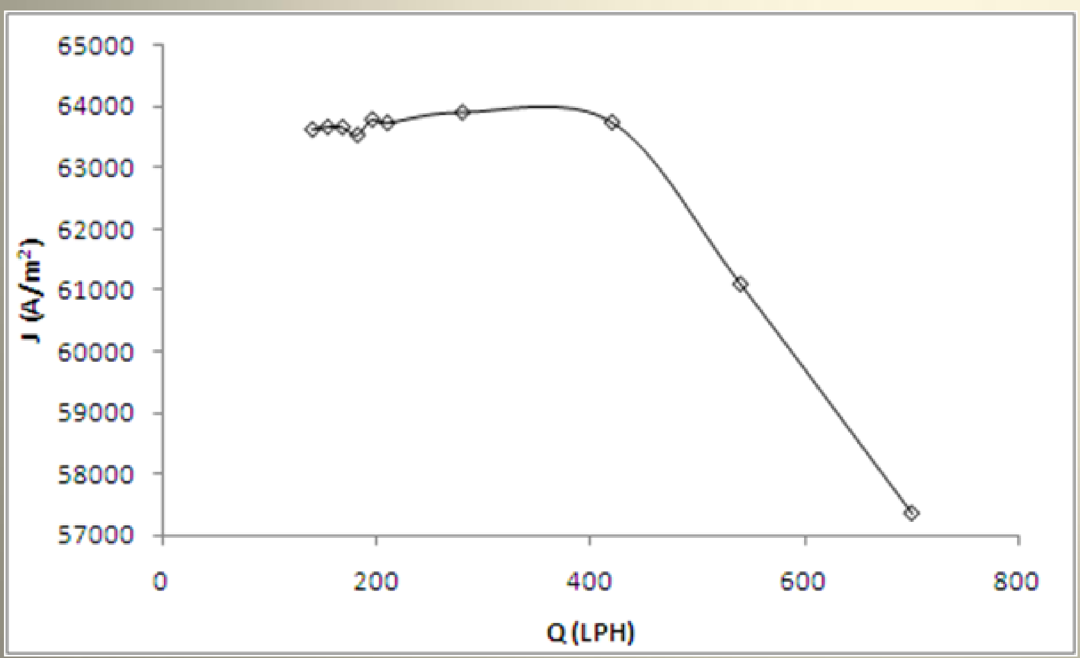
Numerical Simulation of Flow Electrolysers

140 LPH

420 LPH

700 LPH





Current density reduces with continued increase in mercury flow rate

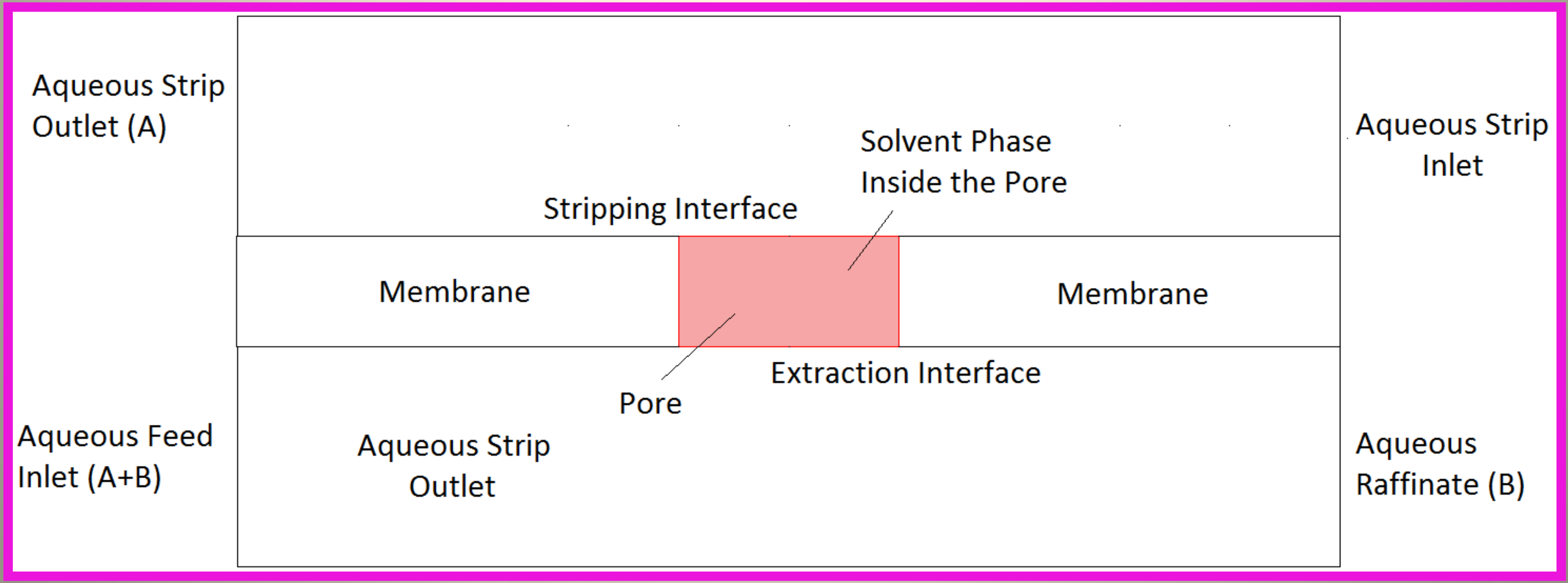
The study provided useful insights into the working of flow electrolysers having streaming mercury cathode

Mass Transfer In a Single Pore of SLM

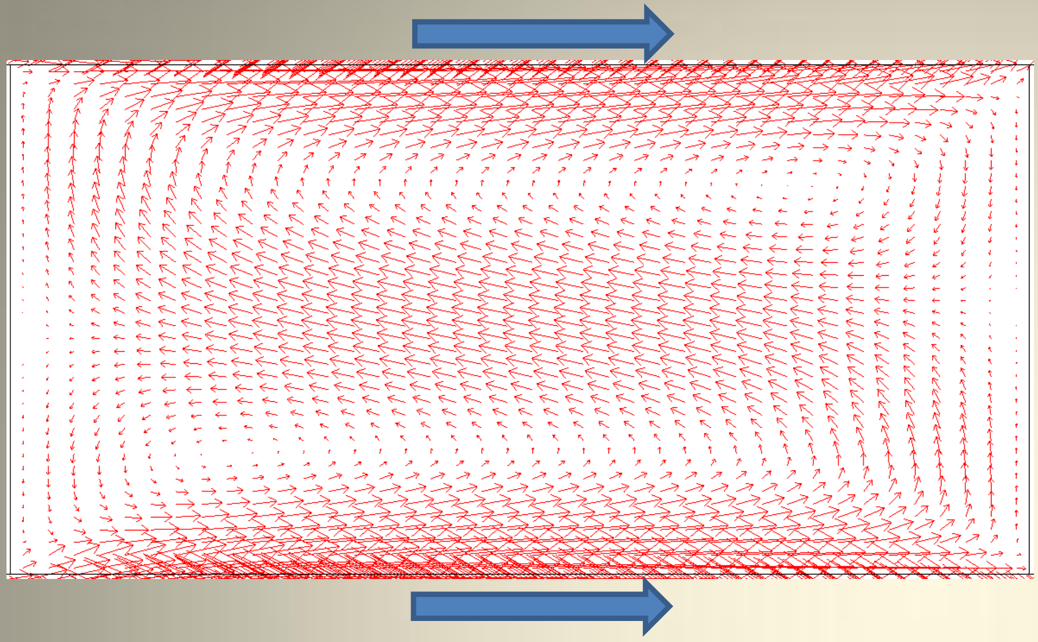
To develop understanding of mass transfer at pore level using numerical simulations and to understand the effects of

- *Flow direction*
- *Physical properties*
- *Pore size*

Coupled solution of Navier-Stokes and Convection-Diffusion equations

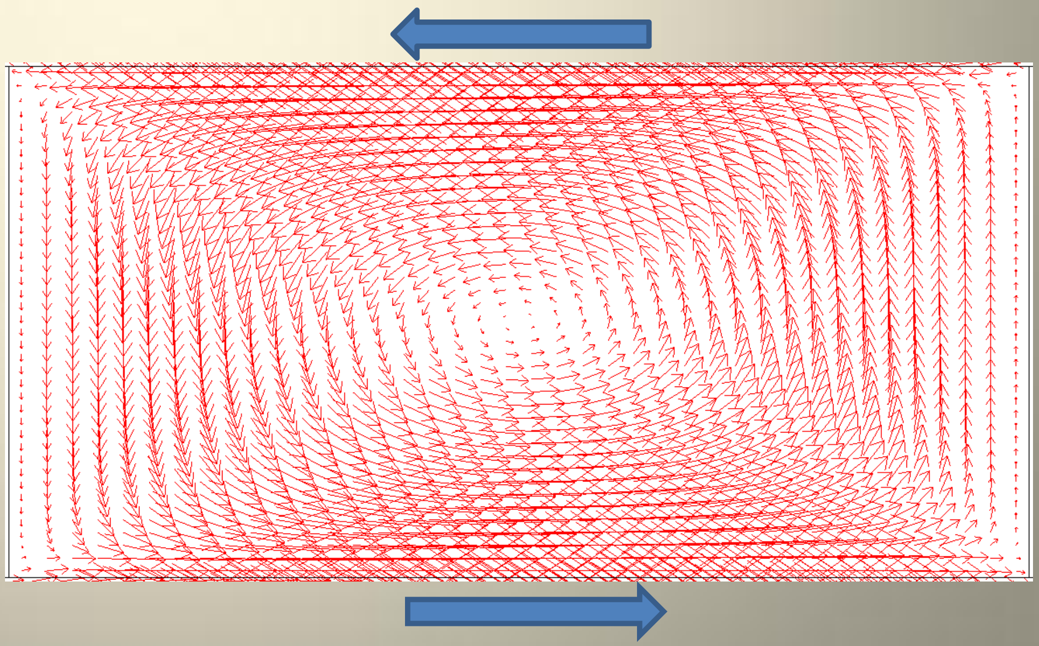


Mass Transfer In a Single Pore of SLM



Two circulation loops

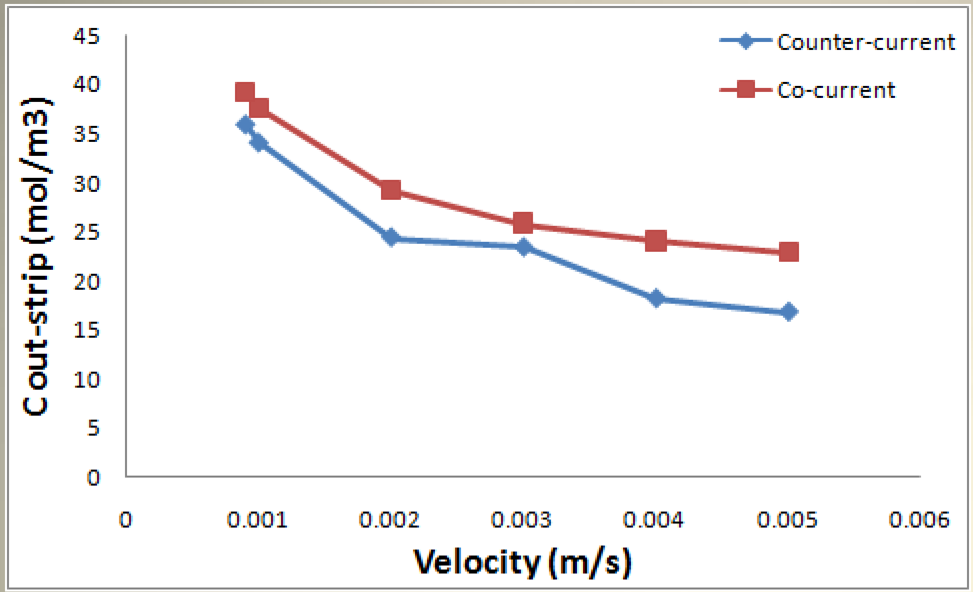
Velocity vectors in the pore for co-current flow



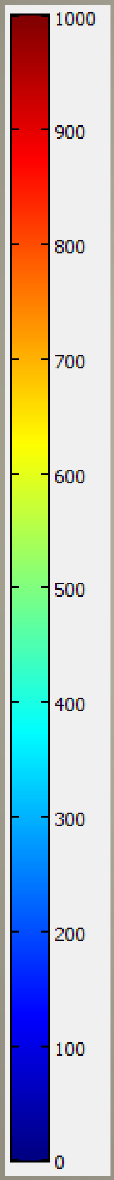
Single circulation loop

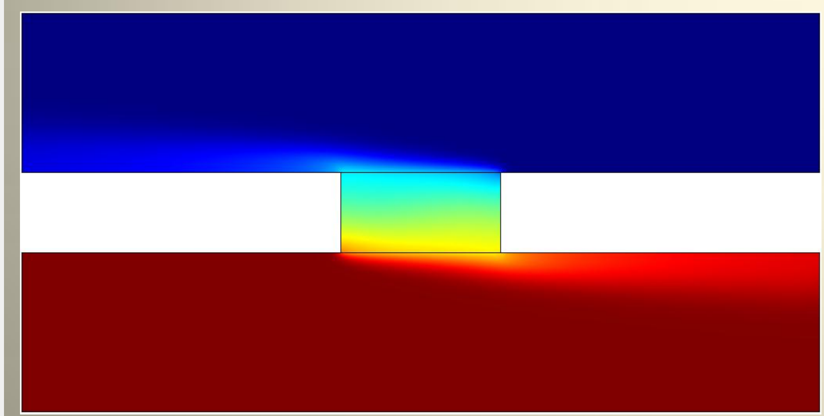
Velocity vectors in the pore for counter-current flow

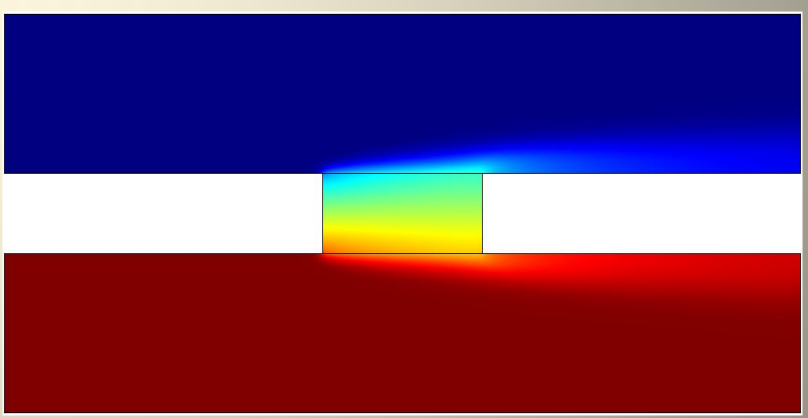
Mass Transfer In a Single Pore of SLM



The study led to an understanding of what happens at pore level in a supported liquid membrane







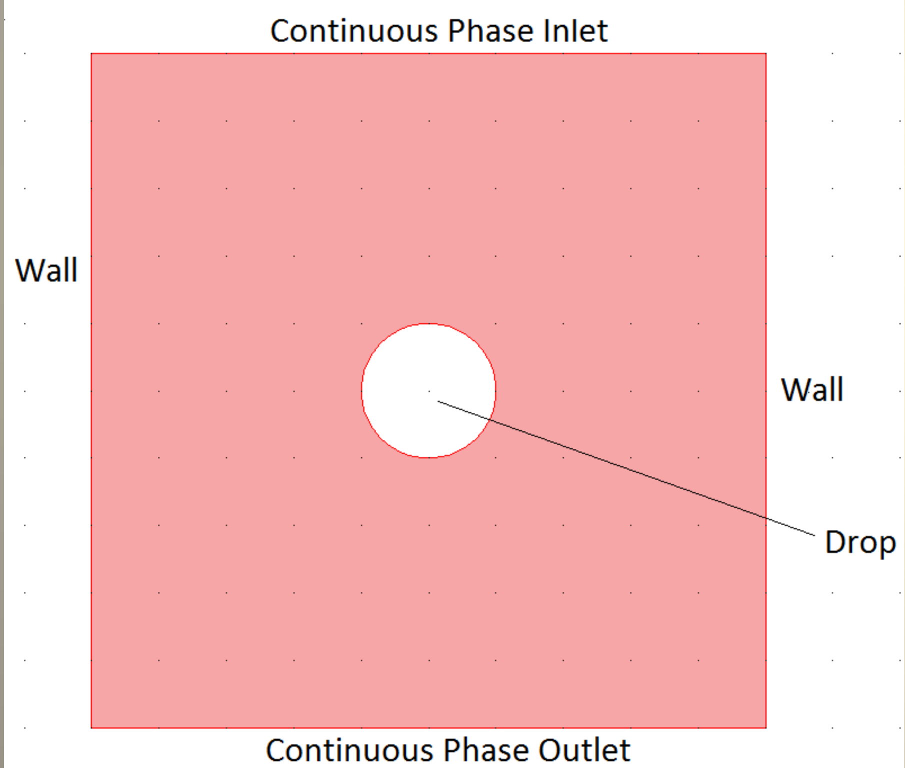
Counter-current flow

Co-current flow

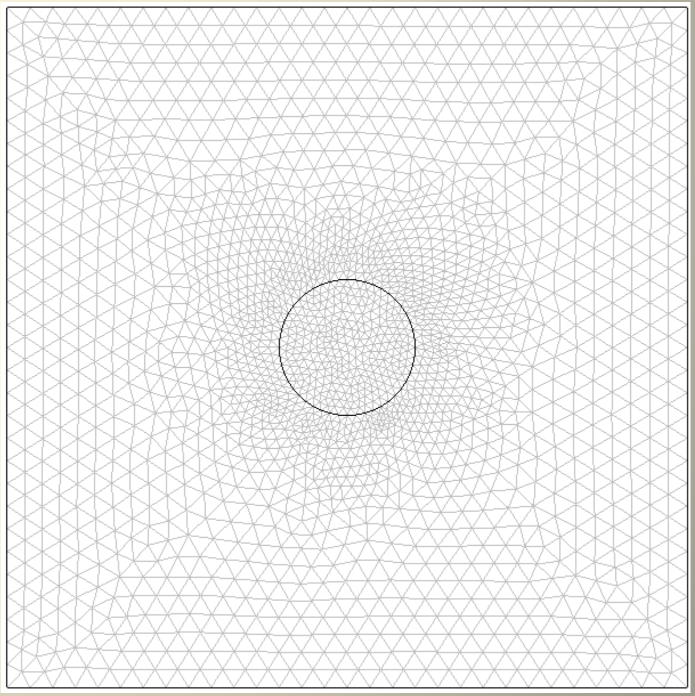
Concentration contours

Mass Transfer For a Single Droplet

- ***Effect of external flow field on internal recirculation inside a drop***
- ***Effect internal recirculation on mass transfer rates***

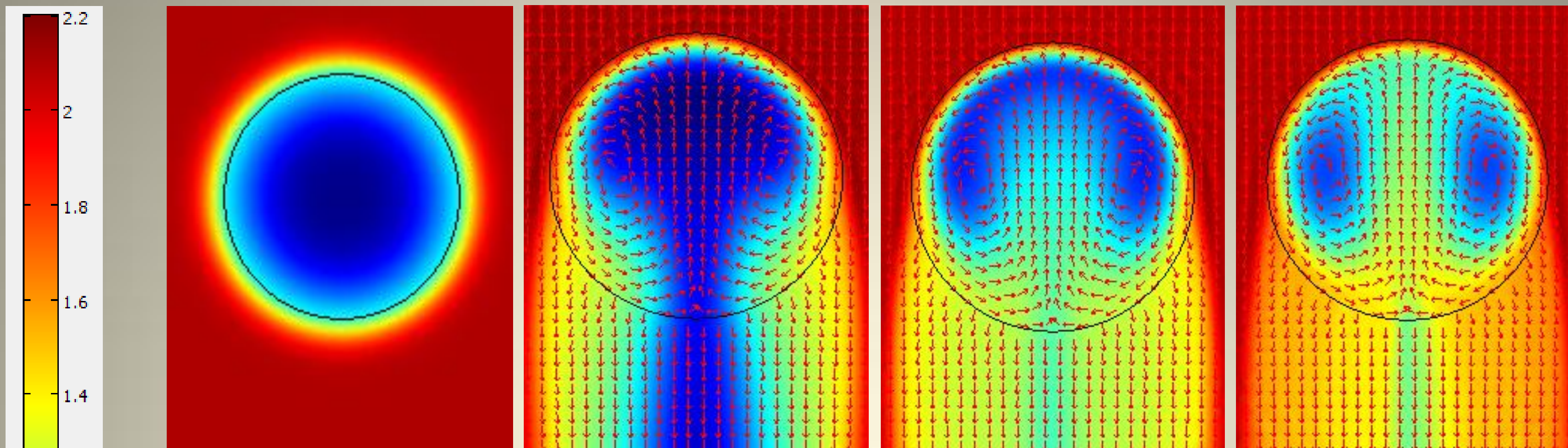


Coupled solution of Navier-Stokes and Convection-Diffusion equations



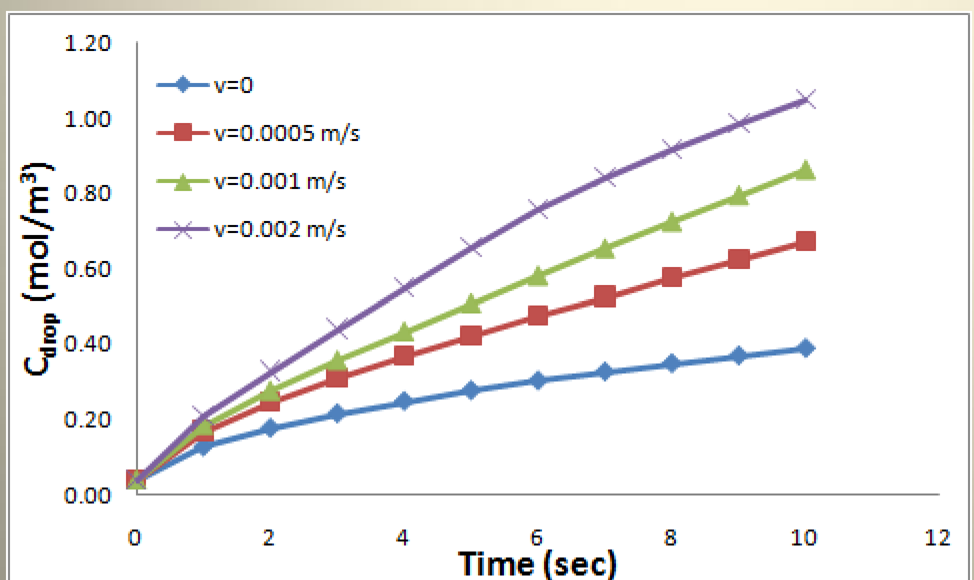
Features like identity boundary conditions etc. were used to implement appropriate boundary conditions at the interface.

Mass Transfer for a Single Droplet



V = 0.0 m/s V = 0.0005 m/s V = 0.001 m/s V = 0.002 m/s

Contours of concentration inside the droplet for different velocities of the external phase



The study shows that internal circulation within a drop and its effect on mass transfer can be captured using simulations carried out in COMSOL multiphysics.

Conclusions

- ***Several interesting application of COMSOL Multiphysics to simulate two-phase flow and multiphysics problems have been presented.***
- ***In some cases results obtained from COMSOL have been quantitatively validated using the experimental data.***
- ***In other cases the results have been qualitatively validated.***
- ***COMSOL Multiphysics is found to be a very useful tool to gain insights into working of process equipment and phenomena involving two-phase flow and multiple physics.***

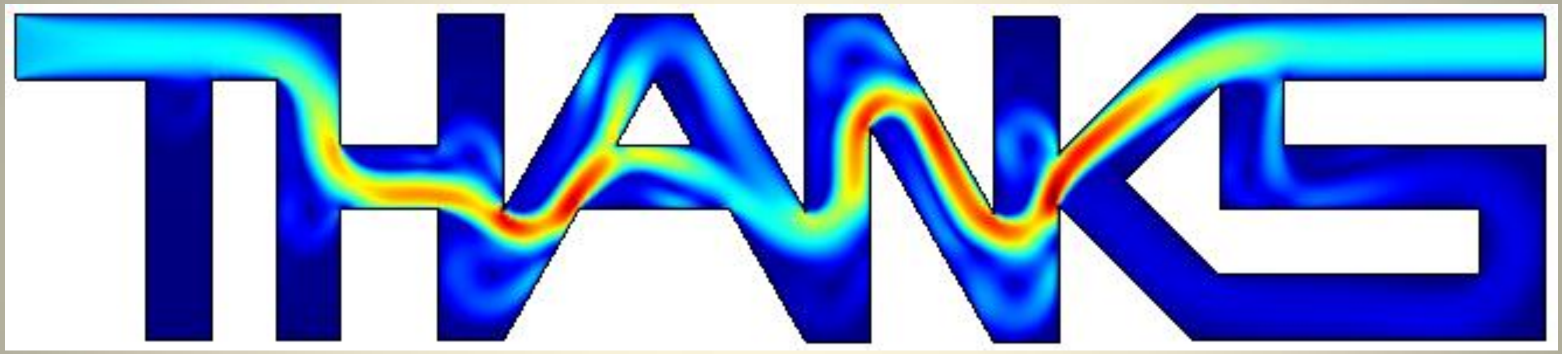
Acknowledgement

Mr. Nirvik Sen, Scientific Officer, Chemical Engineering Division, BARC

Drop formation at a single hole in a sieve plate

Ms. Pragati Shukla, Scientific Officer, Alkali Metal Section, BARC

Numerical simulation of flow electrolysers


THANKS