INSTITUT PIERRE-GILLES DE GENNES
Pour la microfluidique

COMSOL CONFERENCE 2015 GRENOBLE

UPMC PARIS UNIVERSITAS

ensc chimie paris

COMSOL 2015 Conference

14 -16 october 2015, Grenoble, France

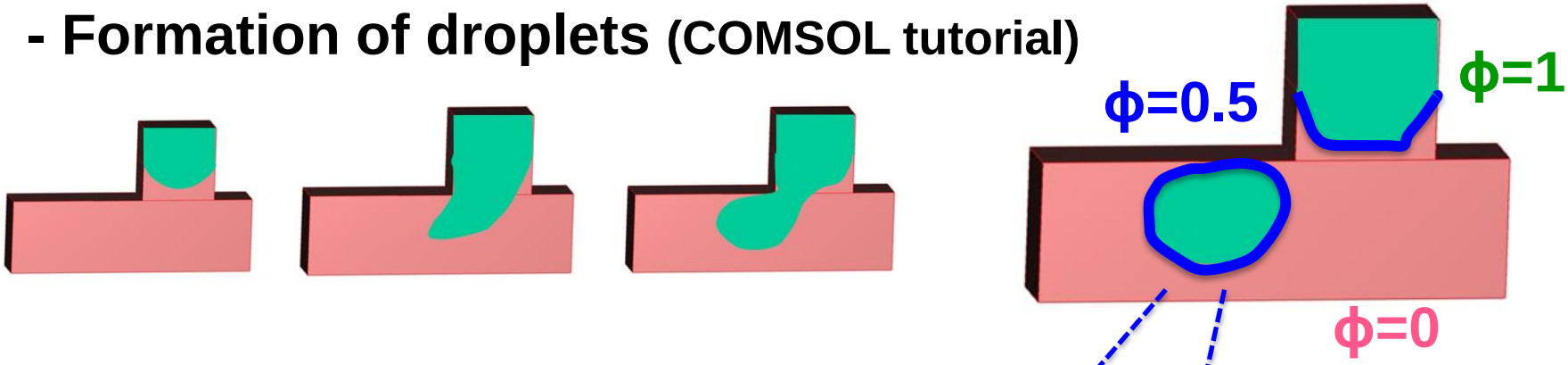
Chemical Reactions at Interfaces during Droplet Formation in Microchannels

Simeon Cavadias [1] , Cédric Guyon [2] , Gerrardo Vera De la Cruz [3]

1 Institut Pierre-Gilles de Gennes (IPGG) - UPMC, France
2 Chimie-ParisTech - Institut Pierre-Gilles de Gennes (IPGG) , France
3 Master Nuclear Energy, ISTN (Saclay), France

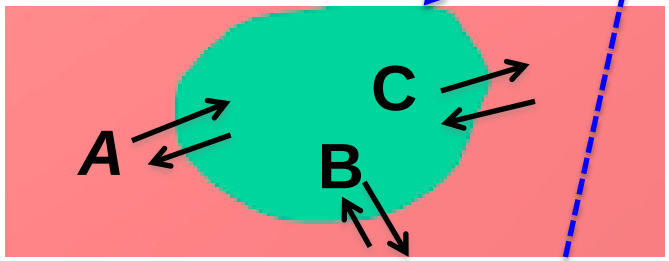
Objective

- Formation of droplets (COMSOL tutorial)



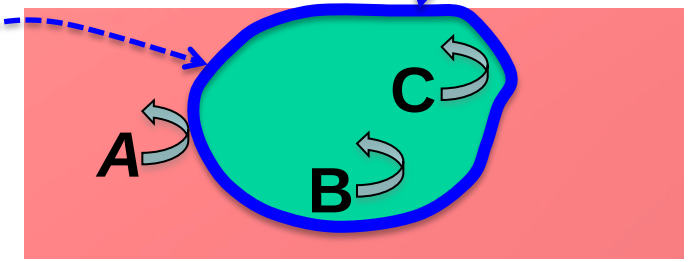
- Reactions inside the droplets $A + B \rightarrow C$

Diffusion of A, B and C in any direction, reaction in any point.



- Reactive extraction $A + B \rightarrow C$

Reaction only at the Interface



Modeling of droplet formation in microchannels

The flow of a 2 phases incompressible fluid is governed by the Navier–Stokes equation:

$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right)-\nabla\cdot\left[\mu\left(\nabla u+\nabla u^{T}\right)\right]+\nabla p=\sigma\kappa n\delta+\rho g$$

$$\nabla\cdot u=0$$

$\sigma\kappa\nu\delta$ describes the surface tension forces and

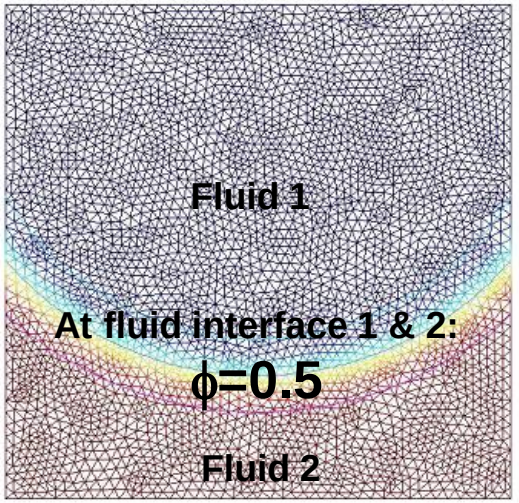
ρg is the gravity force

The interface between the two phases is obtained solving the ϕ in the "Set level model".

$$\frac{\partial\varphi}{\partial t}+u\cdot\nabla\varphi=\gamma\nabla\cdot\left(-\varphi(1-\varphi)\frac{\nabla\varphi}{|\nabla\varphi|}+\varepsilon\nabla\phi\right)$$

where **γ** and **ε** are reinitialization parameters (**ε** determines the thickness of the layer around the interface where **ϕ** changes from 0 to 1, **γ** determines the amount of reinitialization).

The isocontour ϕ = 0.5 determines the position of the interface.
ϕ is transported and reinitialized by the equation:



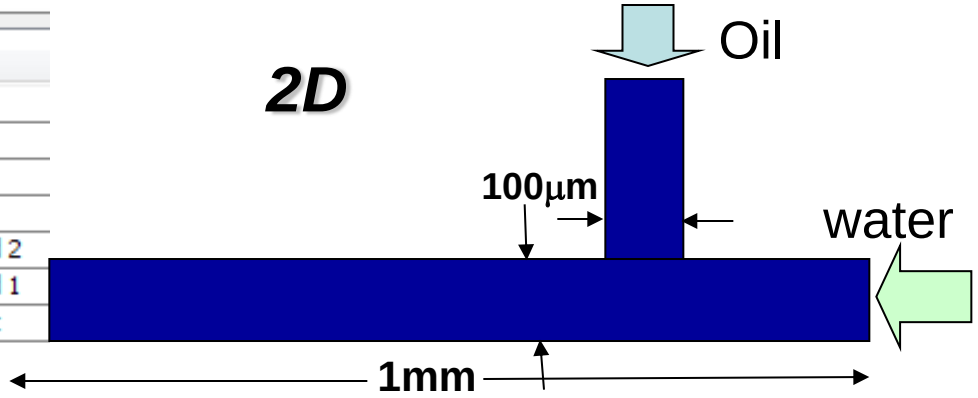
Density and Viscosity

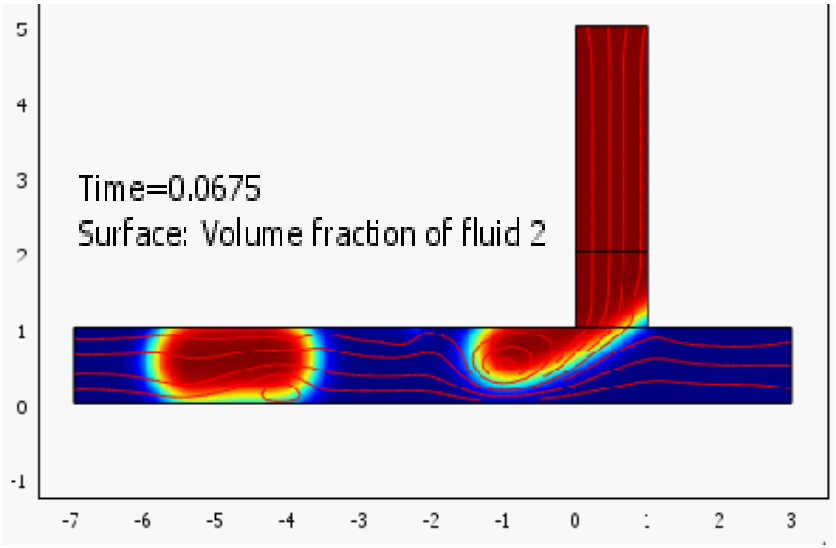
$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$
$$\eta = \eta_1 + (\eta_2 - \eta_1)\phi$$

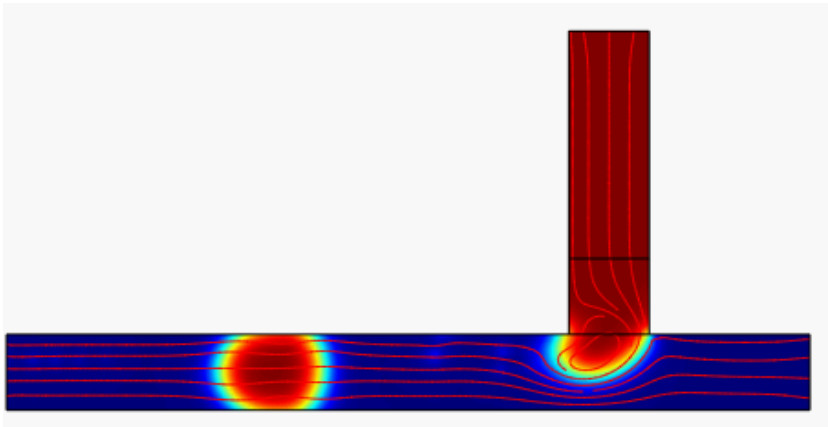
Modeling of droplet formation in microchannels

Constants

Name	Expression	Value	Description
rho1	1e3[kg/m^3]	1000[kg/m^3]	Density, Fluid 1
eta1	1.95e-3[Pa*s]	0.00195	Viscosity, Fluid 1
rho2	1e3[kg/m^3]	1000[kg/m^3]	Density, Fluid 1
eta2	6.71e-3[Pa*s]	0.00671	Viscosity, Fluid 1
uin1	2*vin2	-0.012[m/s]	Maximum inlet speed, Fluid 2
vin2	-0.006[m/s]	-0.006[m/s]	Maximum inlet speed, Fluid 1
sigma	5e-3[N/m]	0.005[N/m]	Surface tension coefficient







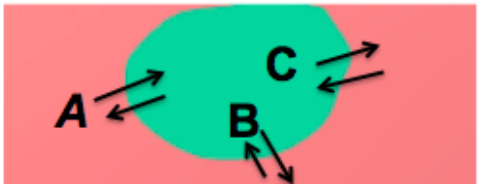
It is possible to reduce the size of the droplets by change of the velocities.

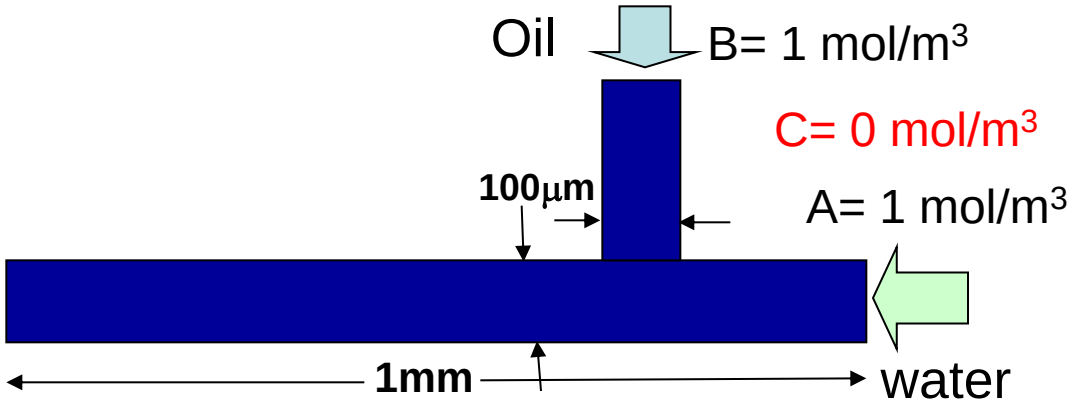
Reactions inside the droplets
and outside

Use of Convection Diffusion (chcd)

$$\delta_{ts}\partial c1/\partial t + \nabla\cdot(-D\nabla c1) = R - \mathbf{u}\cdot\nabla c1,\ c1 = \text{concentration}$$

Diffusion of A, B and C in any direction, reaction in any point.





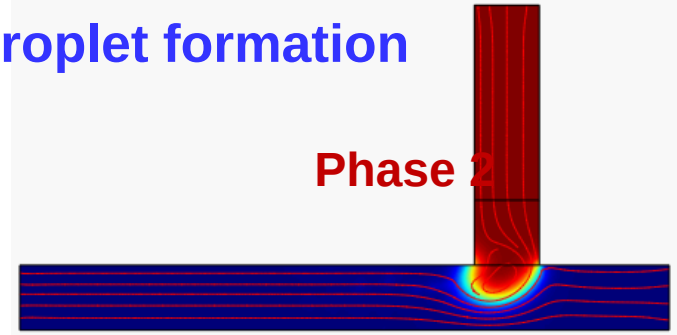
Diffusion coefficient (for A, B and C): 1e-9 m/s^2

R_A=-10*A*B R_B=-10*A*B R_C=10*A*B

Reactions inside the droplets

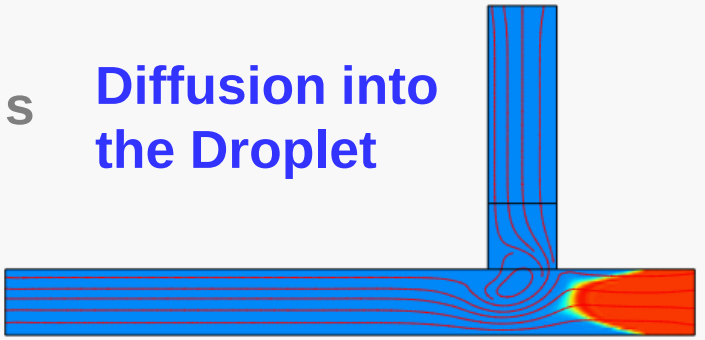
and outside

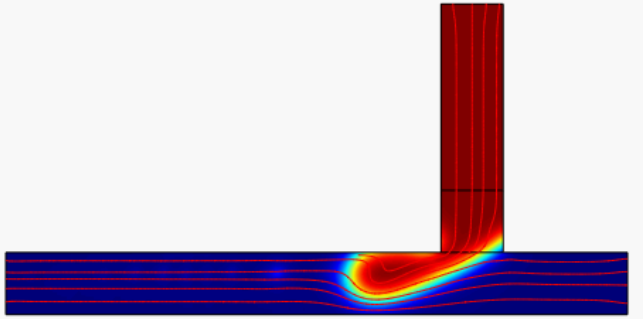
Droplet formation



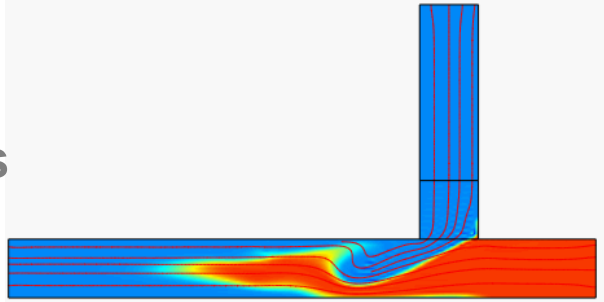
Time: 0.25 s

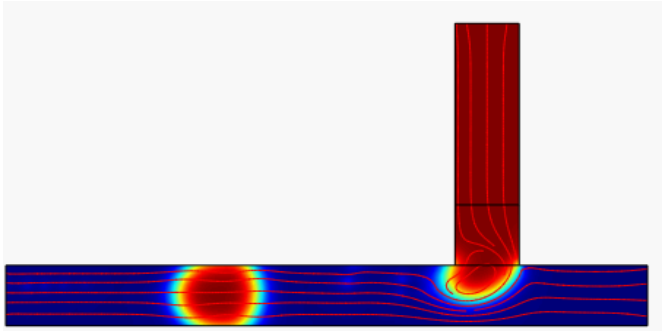
Diffusion into the Droplet



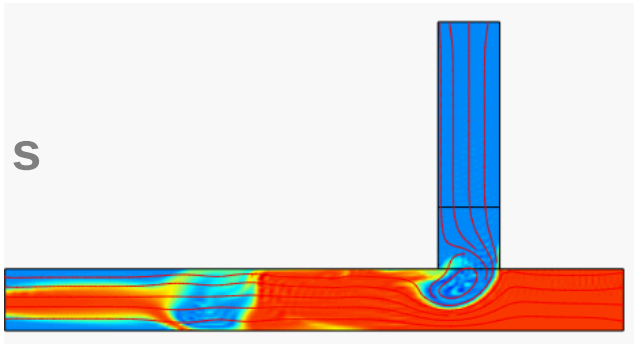


Time: 0.35 s



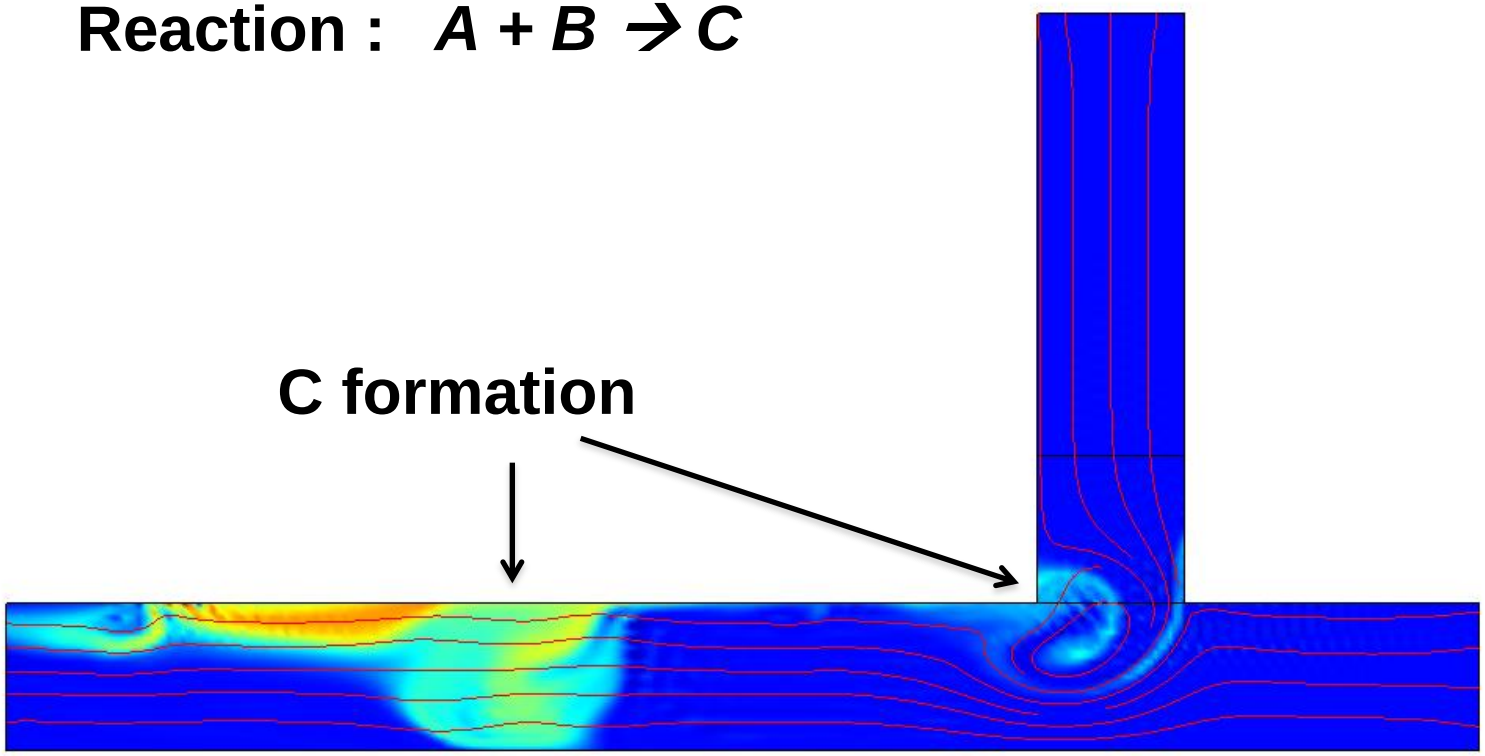


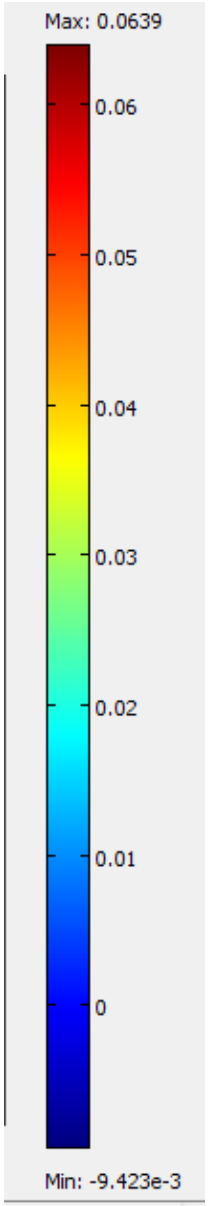
Time: 0.45 s



Reactions inside the droplets
and outside

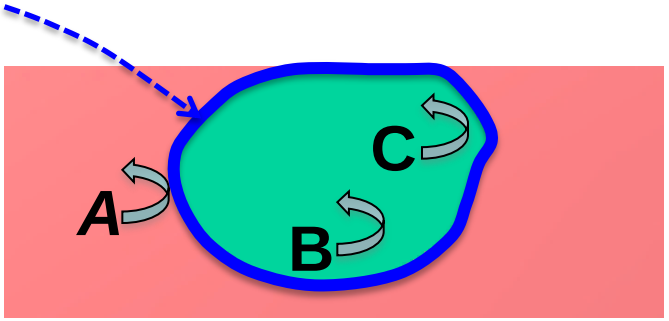
Reaction : $A + B \rightarrow C$





Reactions at the interface of the droplets

Reaction : $A + B \rightarrow C$



Condition in the Diffusion coefficients

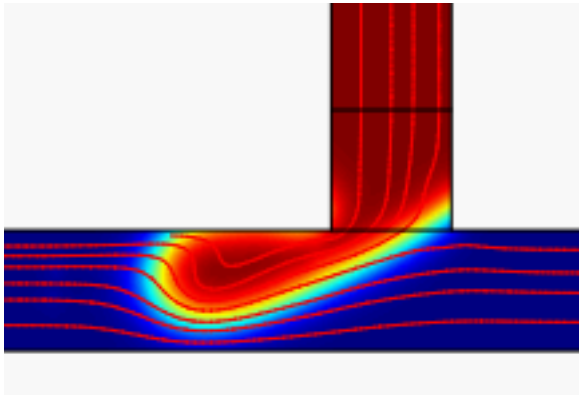
Quantity	Value/Expression	Unit	Description
δ_{ts}	1		Time-scaling coefficier
D (isotropic)	if(phi<=0.6,1e-9,0)[	m^2/s	Diffusion coefficient
D (anisotropic)	1 0 0 1	m^2/s	Diffusion coefficient

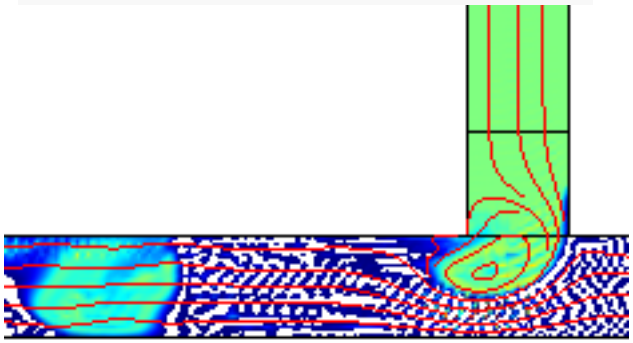
if(phi<=0.6,1e-9,0)[m^2/s]

Condition in the Reaction:
Reaction if $0.4 < \phi < 0.6$

R	if(0.4<=phi&&phi<=	$mol/(m^3 \cdot s)$	Reaction rate
u	u		
v	v	m/s	y-velocity

if(0.4<=phi&&phi<=0.6,-1.0*c1*c2,0)





Problem

Small instabilities (concentrations >1 or <0) accumulated and amplified with the time

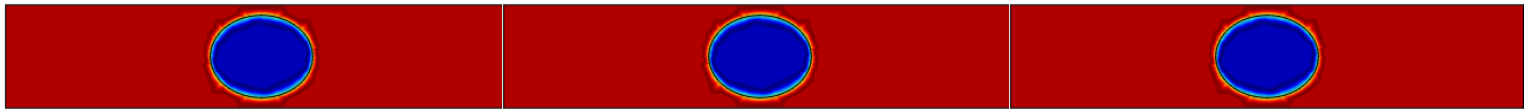
Diffusion versus Reaction

(limiting step, design of the reactor)

Once the droplets formed their size and shape does not change. Microreactors (handreds of microns wide) can have several centimeters length.

The length of the reactor depends on Diffusion/Kinetics

Each drop with the surrounding continuous phase is considered as a batch reactor inside a tubular reactor (plug flow reactor)

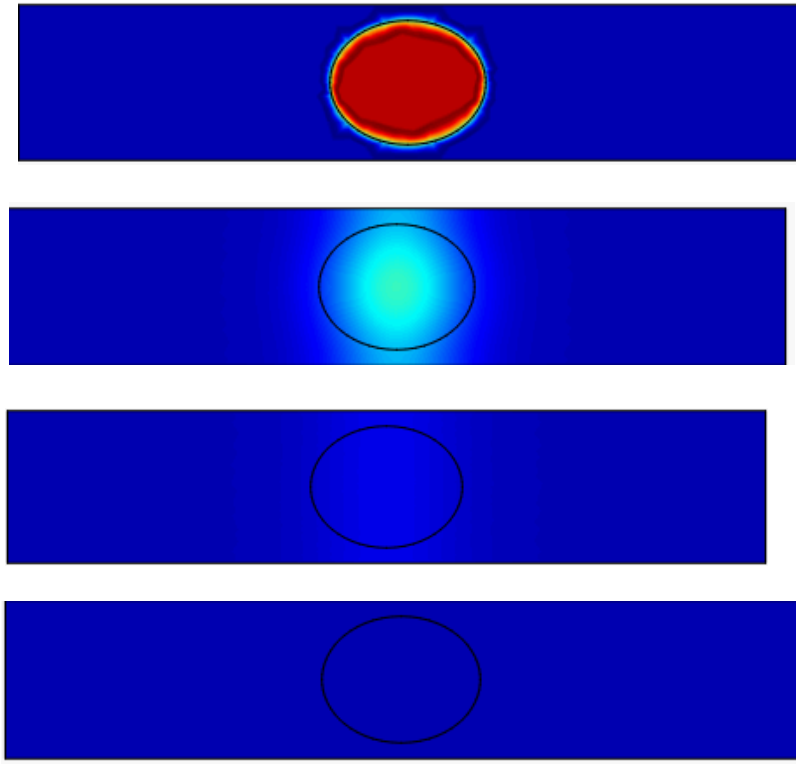


D (isotropic)	if(phi>=0.8,1e-9,0)	m^2/s	Diffusion coefficie
D (anisotropic)	1 0 0 1	m^2/s	Diffusion coefficie
R	if(0.4<=phi&&phi<=	$mol/(m^3 \cdot s)$	Reaction rate
u	0	if(0.4<=phi&&phi<=0.6,-1.0*Aq*Org,0)	

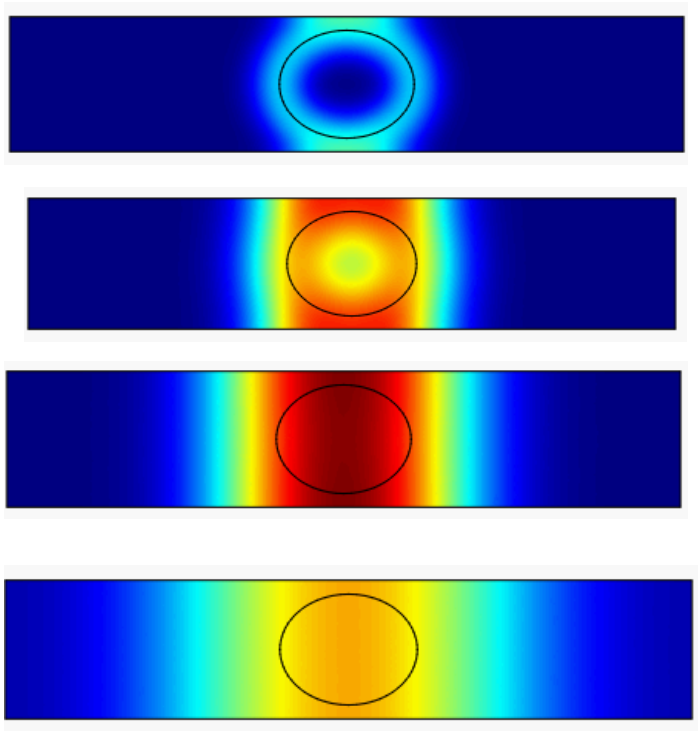
Diffusion versus Reaction

(limiting step, design of the reactor)

Concentration of Org



Concentration of C



As the droplet is small Org decreases rapidly

Conclusion

- **It is possible to simulate in 2D, a droplet formation with different sizes.**

- **It is possible to perform reactions inside the droplets and change their chemical characteristics .**

- **It is possible to perform an optimal design of a microreactor.**

Thank your for your attention

Questions?