Computational Fluid Dynamics : Basics of modelling

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What is Computational Fluid Dynamics ?

- Fluid (gas and liquid) flows are governed by partial differential equations (PDE) which represent conservation laws for the mass, momentum, and energy

$$\rho \frac{Du}{Dt} = -\nabla p + \mu \nabla^2 u + \rho g$$

- Computational Fluid Dynamics (CFD) consist in replacing PDE systems by a set of algebraic equations which can be solved using computers.

Why CFD ?

- To predict properties (velocities, concentration, temperature, electrical field …) in the 3D and with time

- To compute fluid flows (meteorogical phenomena, transport of contaminant, combustion) but also :
  - Human body (blood flow, breathing …)
  - Biomedical devices

➡ After validation, CFD simulations can be considered as « Numerical experiments »

How to do CFD ?

Commercial codes

Can handle complex geometries and multiphysics problem

Can produce accurate solutions

Open source code

Python (programming language) + SciPy (eq. To Matlab)

+ FiPy (finite volume PDE solver)

Available on the ENTHOUGHT SCIENTIFIC COMPUTING SOLUTIONS canopy platform

From 80's the code evolves to easy to use software

But should be used with care by users (with a good knowledge and expertise)

http://www.ansys.com/

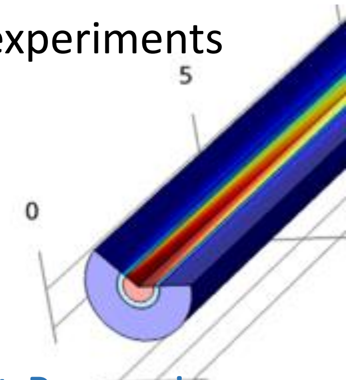
http://www.comsol.com/

http://www.scipy.org

http://www.ctcms.nist.gov/fipy

How to do virtual experiments of the real world with CFD ?

Engineering		*Physics – Chemistry*		*Mathematics*		*Computation*		*Engineering*	
Real world	→	Conceptual model	PDE →	Computer model Numerical recipes (discretization techniques) Cf Efrem course	→	Post-processing	→	Validated numerical experiments



1 Pre-processing

Model providing acceptable level of complexity ?

2 Processing

Will be presented here as a recipe (consider a preparation time of 1 day) !

3 Post-Processing

Accurate representation of reality ?

1 Pre-processing

Formulate the model

Real world → Conceptual model

Expertise for the model statement

Objectives : Conceptual model providing acceptable depicting of the targeted application

Need an engineering approach of the problem

- What are the objectives (variable to determine) ?
- What is the simplest (but not simpler) way to describe the problem ?
- What is (are) the limiting phenomena ?
- What physical phenomena have to be accounted ?
  - Coupling of fluid mechanics, heat transfer, mass transfer ?
    - Simplification of the flow -> Poiseuille flow
  - Geometry of the domain
    - Possible simplification
    - Simplification of the geometry 3D->1D
- What would be the way to progress from the simplest simulation to the final one ?

Prerequisite on transport phenomena

What?

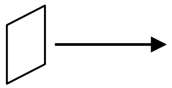
Transport		
Energy		Mass
mechanical	thermal	

Flux transported per time unit and sectional area

How many ?

Momentum flux	Heat flux	Mass flux
τ	Q	N
$\frac{kg.m.s^{-1}}{m^2.s}$	$\frac{J}{m^2.s}$	$\frac{mol\ ou\ kg}{m^2.s}$
Shear stress		
Force per area		

?



Fluid mechanics	Heat transfer	Mass transfer
Transport by potential gradient		Diffusion
Shear rate **Newton law** $\tau_{yx} = -\mu \frac{du_x}{dy}$ **viscosity**	Temperature gradient **Fourier law** $Q = -\lambda \frac{d\theta}{dx}$ **Thermal conductivity**	Concentration gradient **Fick law** $N = -D \frac{dc}{dx}$ **diffusion**
Transport by advection u * quantity/m^3		Advection
$u\rho u$	$Q = uC_p\rho(\theta - \theta_{ref})$	$N = uc$
Transport due to external forcing		
Pressure, Gravity	Radiation	Electrical field …
Transformation : source or sink term		
	Chemical, electrical or mechnical energy	Homogeneous reaction $r = \frac{1}{V}\frac{dn}{dt} = kc$

How ?

When and where ?

Fluid mechanic	Heat transfert	Mass transfer
u = f (x,y,z,t) τ =f (x,y,z,t)	θ = f (x,y,z,t) Q =f (x,y,z,t)	c = f (x,y,z,t) N =f (x,y,z,t)

Conservation law :

accumulation = inlet- outlet +- source term

Continuity equation

$$div(\rho\vec{u}) = 0$$

Momentum balance

$$\rho\frac{Du}{Dt} = -\nabla p + [\nabla \bullet \tau] + \rho g$$

$$= -\nabla p + \mu\nabla^2 u + \rho g$$

$$\frac{kg.m.s^{-1}}{m^3.s}$$

(Navier-Stokes)

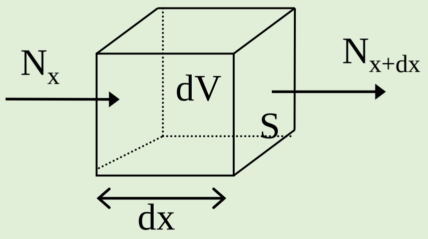
$$\rho C_p \frac{d\theta}{dt} = -div(\vec{Q}) \pm s$$

$$J.m^{-3}.s^{-1}$$

$$\frac{dc}{dt} = -div(\vec{N}) \pm r$$

$$mol.m^{-3}.s^{-1}$$

Development in 1D in Cartesian coordinates



Accumulation = Inlet - outlet +- reaction

dV dc = S N_x.dt - S N_{x+dx} dt + r S dx

$$\frac{dc}{dt} = -\frac{dN}{dx} \pm r$$

Expert system for PDE writing

Coordinates ?

Cartesian | Cylindrical | Spherical

Dimension ?

1 | 2 | 3

Steady state ? **Transient ?**

Source term (chemical reaction) ?

Yes | No

Transfer mode ?

Diffusion | Advection | Mix

Partial differential equation for the concentration max order 1 for time and order 2 for spatial direction

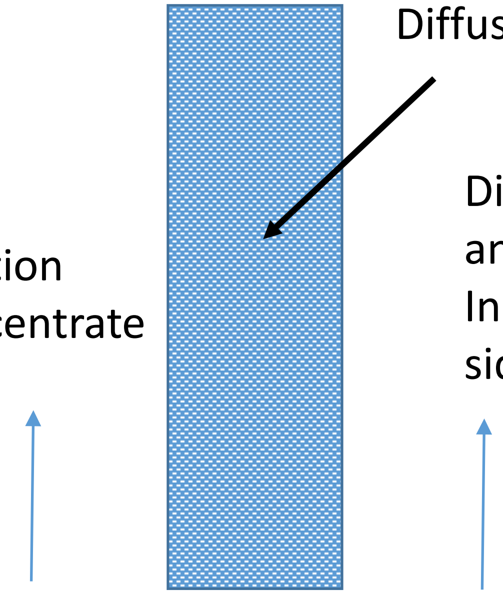
Initial condition ? $t=t_0$ $c=c_i$

Boundary conditions ? $x=x_0$ $c=c_0$, $N=N_0$, $dc/dx=0$

Concentration profile And mass flux

Exemple of dialysis modeling

1D cartesian model of dialysis



Should Be Made as Simple as Possible, But Not Simpler

Diffusive transport in the membrane

Diffusive transport
Steady state

coordinate ?

cartesian

Direction ?

1 | 2 | 3

Steady state? | **Transient?**

Source term ?

No | Yes

Transport mode ?

diffusion | advection

Cartesian Conservation law

$$\cancel{\frac{dc}{dt}} = -\frac{dN}{dx} \pm \cancel{r}$$

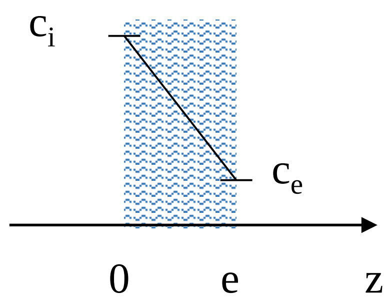
Steady state? **1** **No**

Diffusive transport

diffusion $N = -D\frac{dc}{dz}$ $D\frac{d^2c}{dz^2} = 0$

B.C. 1 x=0 $c=c_i$

C.L. 2 x=e $c=c_e$



$$\frac{c-c_i}{c_e-c_i} = \frac{z}{e}$$

$$NS = S\frac{D}{e}(c_i - c_e) = \frac{c_i - c_e}{\frac{e}{DS}}$$

Diffusion transport resistance

Diffusive-Advection at interface

Diffusion and advection at interface

Coordinates ?

cartesian

Direction ?

1 **2** 3

Steady state

Transient

Souree term ?

No

Yes

Transport mode ?

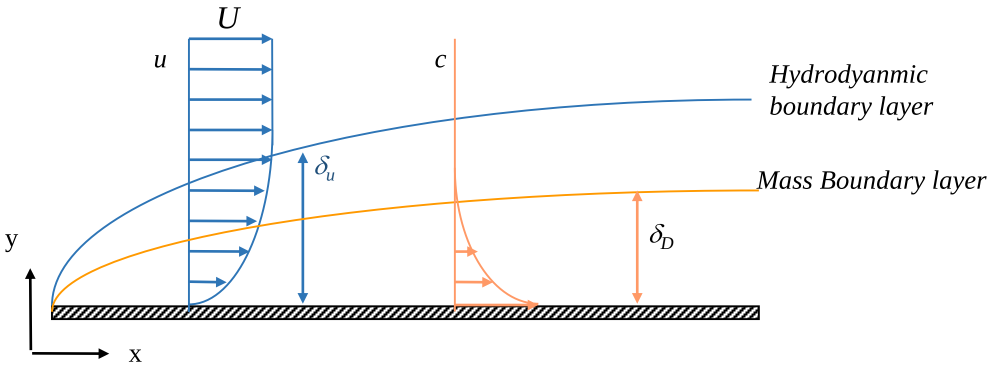
diffusif

convectif

$$\frac{dc}{dt} = -\left[\frac{dN_x}{dx} + \frac{dN_y}{dy}\right] \pm R$$

$$\cancel{\frac{dc}{dt}} = D\left[\cancel{\frac{d^2c}{dx^2}} + \frac{d^2c}{dy^2}\right] - \left[u_x\frac{dc}{dx} + \cancel{u_y}\frac{dc}{dy}\right] - c\left[\cancel{\frac{du_x}{dx} + \frac{du_y}{dy}}\right] \pm \cancel{R}$$

$$div(\rho\vec{u}) = 0$$



Boundary layer : thickness of fluid where the gradient is localised

Simplified tool for engineers

Mass transfer coefficient, k

$$N = k(c_i - c_b)$$

m/s

Concentration at interface

$$\boxed{k = \frac{D}{\delta_D}}$$

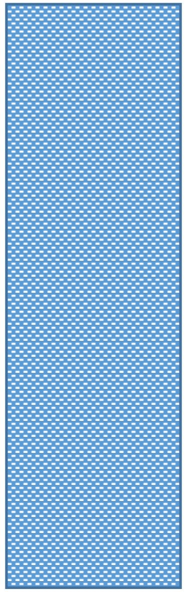
Dimensionless correlation

$$Sh = 1{,}86\left(Re.Sc.\frac{d_H}{L}\right)^{0{,}33} \quad Re<2100$$

1D dialysis conceptual modeling

$$N = \frac{D}{e}\left(c_{ci} - c_{di}\right)$$

$$N = k_c\left(c_c - c_{ci}\right)$$



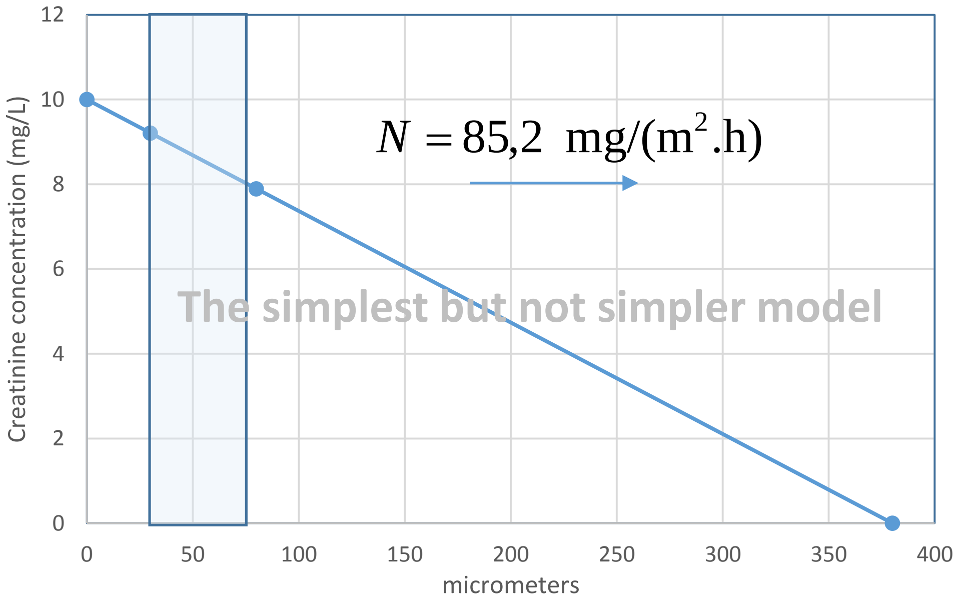
$$N = k_d\left(c_{di} - c_d\right)$$

Diffusion
and advection
In the concentrate
side

Diffusion
and advection
In the dialysate
side

$$N = \frac{\left(c_c - c_d\right)}{\frac{1}{k_d} + \frac{e}{D} + \frac{1}{k_c}}$$

Diffusion of creatinine 910-10 m2/s
Boundary layer in concentrate 30 μm
Boundary layer in dialysate 200 μm
Membrane thickness 50 μm



The start point before CFD

The establishment of the conceptual model is a key point :

- to know the physics to inject in simulations
- to understand the mechanisms (and then to interpret the simulation results)

Cf Dmytro work

The simplest model can then be refined :

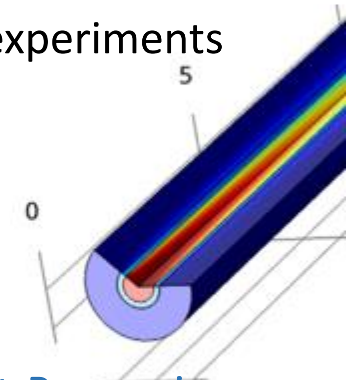
➡ More complex physics : partition coefficient, reactive layers (adsorption, biological …)

➡ More realistic : other geometries, 2D, 3D (need CFD)

How to do virtual experiments of the real world?

Engineering		Physics – Chemistry		Mathematics-Computation		Engineering	
Real world		Conceptual model	PDE	Computer model		Post-processing	Validated numerical experiments

Numerical recipes
(discretization techniques)
Cf Efrem course



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3 Post-Processing

Accurate representation of reality ?

2 Processing

Perform simulation

Conceptual model → Computer model → Post-processing

The way to do : from an example

- Follow a complicated recipes (integrating sequentialy the ingredients)

- Perform simulation

- Change the ingredients and the operating conditions –Redo simulations

BIO ART

Modeling Instructions X 30

From the **File** menu, choose **New**.

NEW

1 In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select physics** tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

3 Click **Add**.

4 In the **Concentrations** table, enter the following settings:

c1

5 In the **Select physics** tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

6 Click **Add**.

7 In the **Concentrations** table, enter the following settings:

c2

8 In the **Select physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

9 Click **Add**.

10 Click **Study**.

Time scale for a superficial learning is days

The way to do : from scratch with a software

- Apply KISS principles : *Keep It as Simple as poSsible, Keep it small and simple, Keep it sober and significant …*

- Define the simplest physics, the smallest geometry
- Perform simulations
- Add new ingredients (one by one)
- Check simulations (save your work with a new file name)
- Be fair with computational time

<u>YOU WILL DO ERRORS</u>
BUT ON SIMPLE AND RAPID SIMULATIONS

Time scale for this learning is months

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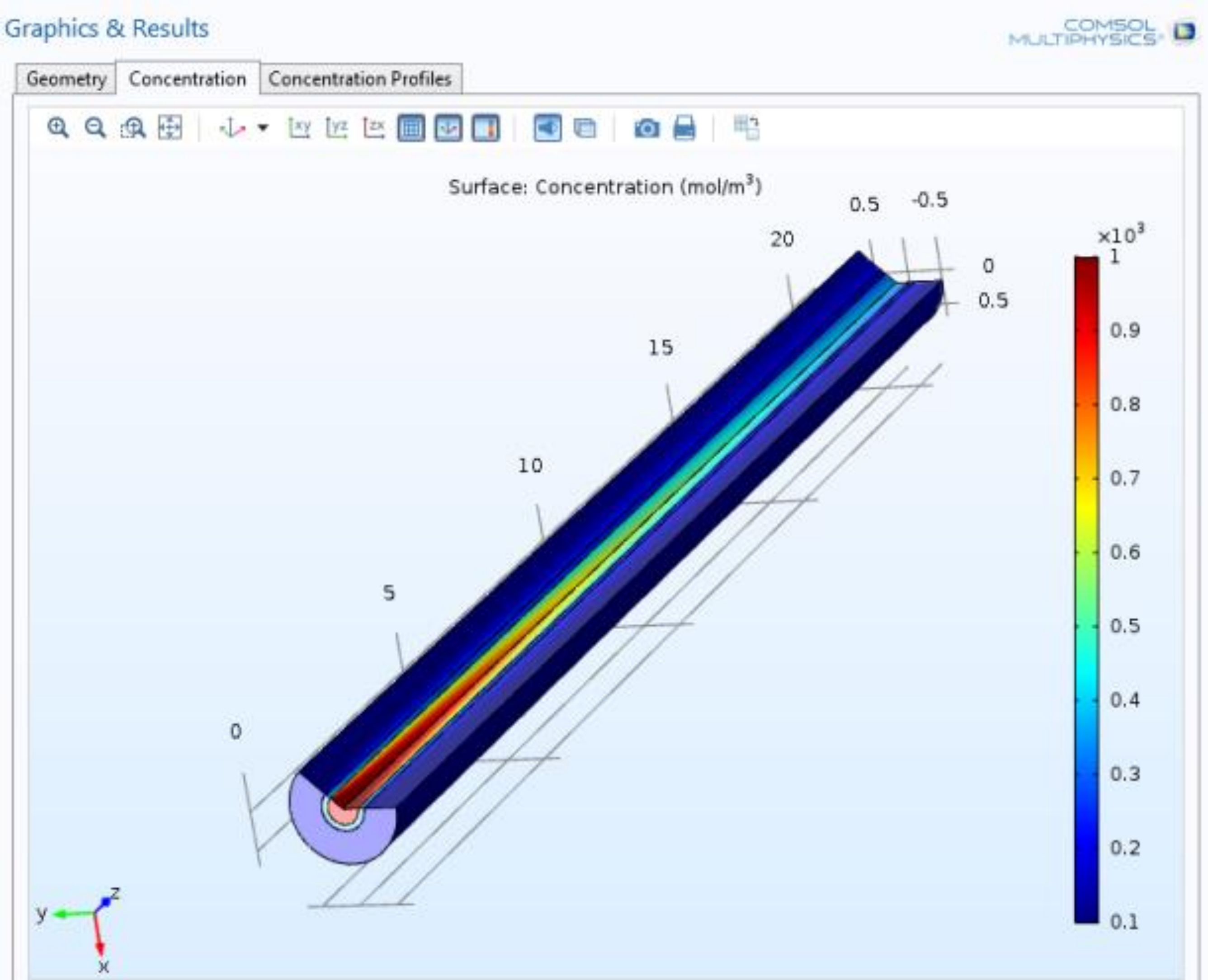
The way to do :
from scratch with a home code

Time scale for a deep learning is years !

```python
#derivative of osmotic pressure -> colloid-colloid interaction induced diffusion
def dPidphi(phi):
  Pii = zeros(len(phi))
  out = zeros(len(phi))
  #calculation of the solid pressure (without transition zone)
  for i in range(len(phi)):
    if phi[i]<=phicrit :
      Pii[i]=(phi[i]*kT/vp)+(aosm*((phi[i])**bosm))
    else :
      Pii[i]=Piosmcrit*((((phicp-phicrit)/(phicp-phi[i])))**(1./comp))

  #calculation of the solid pressure derivative
  for i in range(len(phi)):
    if phi[i]<=phicrit :
      out[i]=(kT/vp)+(aosm*bosm*((phi[i])**(bosm-1.)))
    else :
      out[i]=Piosmcrit*((1./comp)/(phicp-phi[i]))*((((phicp-phicrit)/(phicp-phi[i])))**(1./comp))
    #application of the transition zone
    out[i]=out[i]*(1.-(irrev*norm.pdf(Pii[i],Piosmcrit,sigma)/norm.pdf(Piosmcrit,Piosmcrit,sigma)))*vp/kT
  return out

def Kphi(phi):
  out = (6.-9.*(abs(phi)**(1./3.))+9.*(abs(phi)**(5./3.))-6.*(abs(phi)**2.))/(6.+4.*(abs(phi)**(5./3.)))
  return out

def diffusion(phi):
  out = Kphi(phi)*dPidphi(phi)
  return out

Pe=u[0]*delta/D0
Pebl=Pe*deltabl1/delta
Pem=Pe*deltam/delta
tdiff=delta*delta/D0
x_1=deltabl1/delta
x_2=(deltabl1+deltaex1)/delta
x_3=(deltabl1+deltaex1+deltam)/delta
x_4=(deltabl1+deltaex1+deltam+deltaex2)/delta
```

From an example :
dialysis simulation with COMSOL Multiphysics



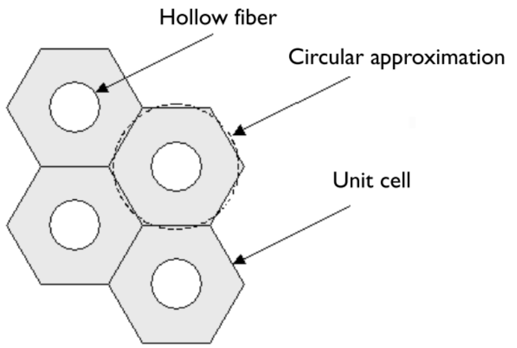
Comsol multiphysics

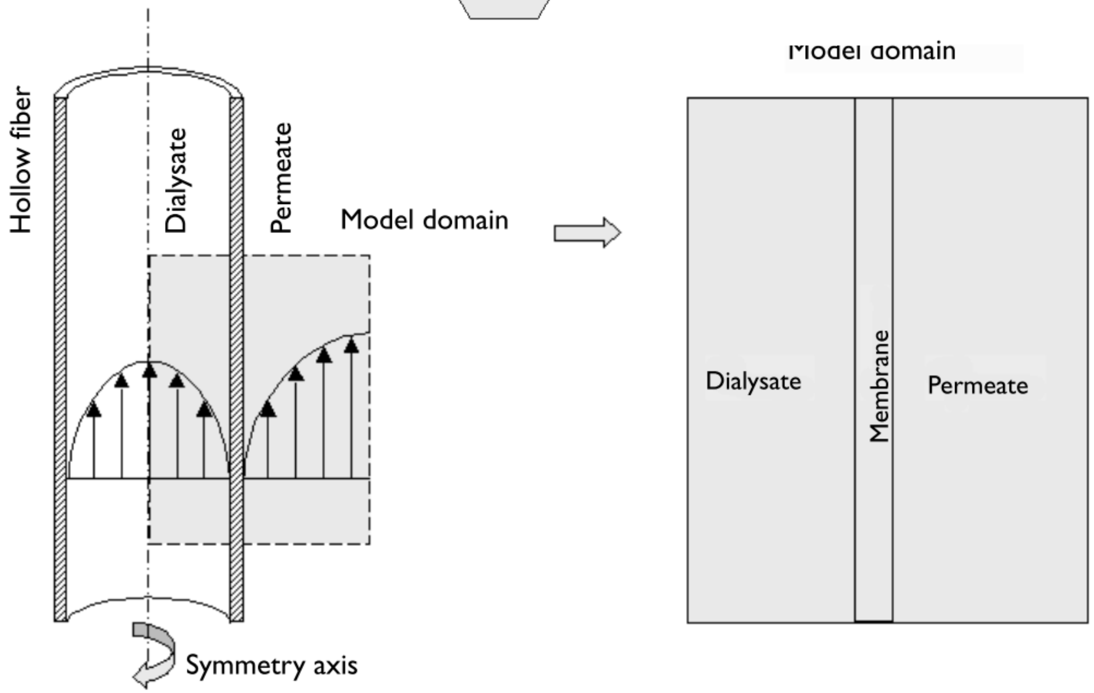
$7995 for a single-user license
$1700 for academics
but a lot of module in option

Options needed for biomedical app.
- CFD module $1700
- Reaction eng. module $800

Ingredients for dialysis

- **Domain**
- Meshing
- Physics model
- Fluid properties
- Boundary conditions
- Calculations
- Post processing





Ingredients for dialysis

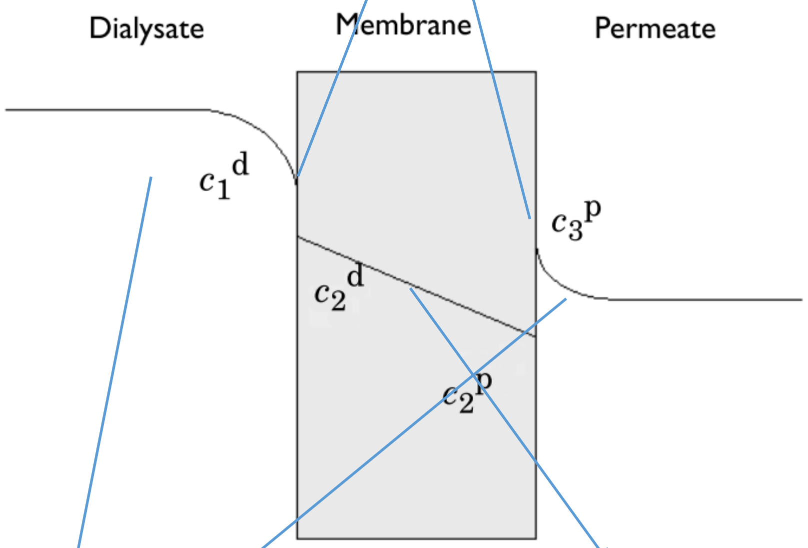
- Domain
- **Meshing**
- Physics model
- Fluid properties
- Boundary conditions
- Calculations
- Post processing

Enough meshes to be accurate
Not too much to save computational time

Ingredients for dialysis

- Domain
- Meshing
- **Physics model**
- Fluid properties
- Boundary conditions
- Calculations
- Post processing

Partition coefficient (equilibrium)



Diffusion in the membrane

Diffusion and advection
-> description of the mass boundary layers

Ingredients for dialysis

- Domain
- Meshing
- Physics model
- **Fluid properties**
- Boundary conditions
- Calculations
- Post processing

PROPERTY	VALUE	DESCRIPTION
D	10^{-9} m^2/s	Diffusion coefficient, liquids
D_{m}	10^{-9} m^2/s	Diffusion coefficient, membrane
R_{hf}	0.2 mm	Inner radius, hollow fiber
L_{m}	0.28 mm	Thickness, membrane
L_{pc}	0.7 mm	Width, concentric permeate channel
H	21 mm	Length, fiber
$U_{\mathrm{ave\_dia}}$	0.5 mm/s	Average velocity, dialysate
$U_{\mathrm{ave\_per}}$	0.8 mm/s	Average velocity, permeate
K	0.7	Partition coefficient
c_0	1 M	Inlet concentration, dialysate

Ingredients for dialysis

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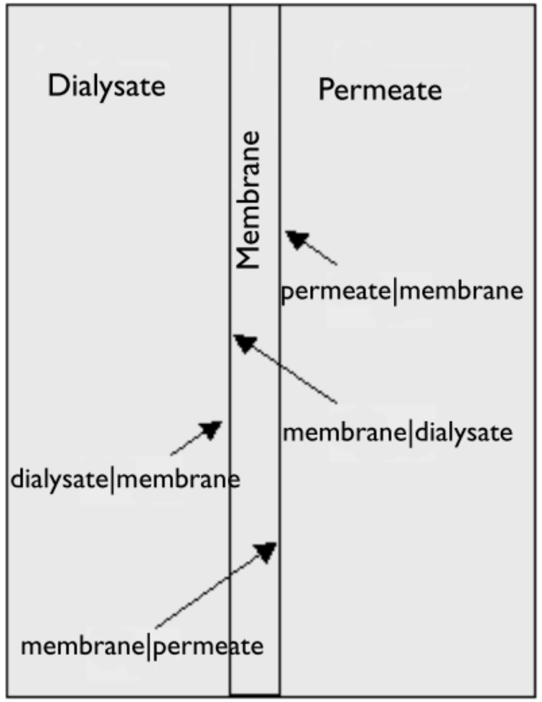
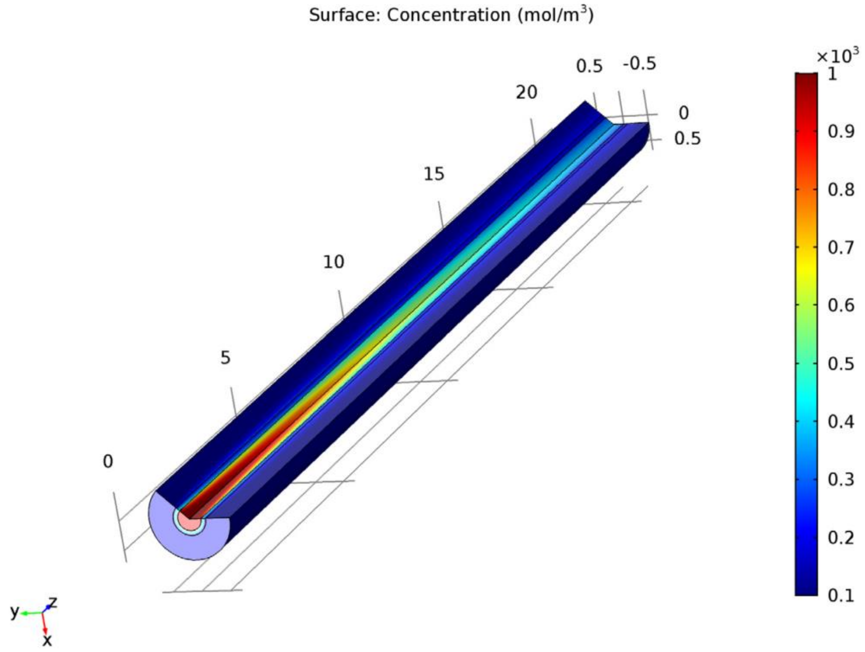
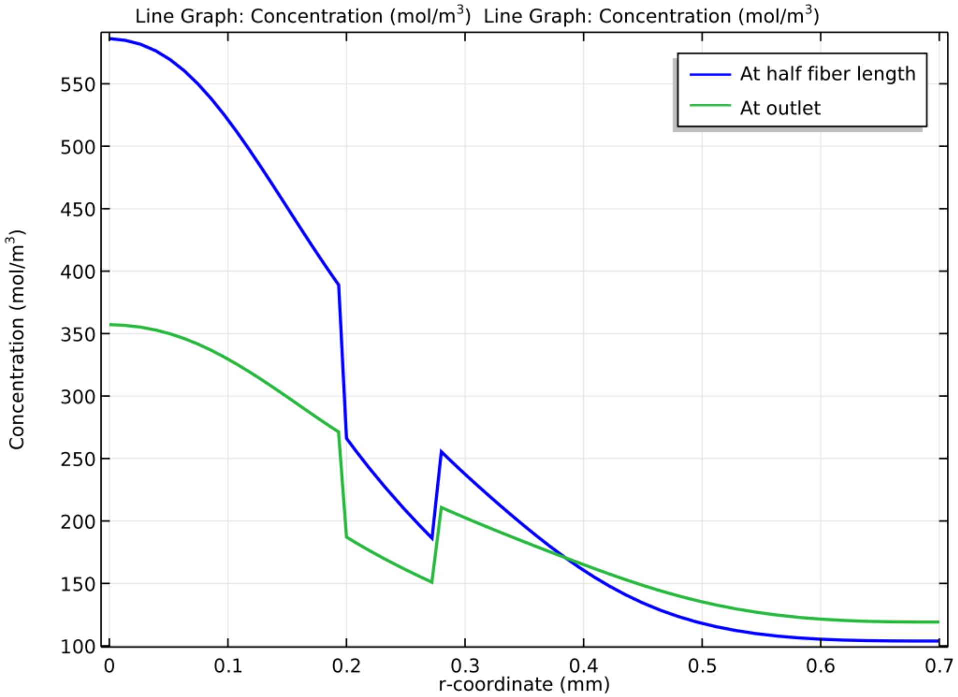


Ingredients for dialysis



- Domain
- Meshing
- Physics model
- Fluid properties
- Boundary conditions
- Calculations
- **Post-processing**



How to do virtual experiments of the real world?

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Numerical recipes
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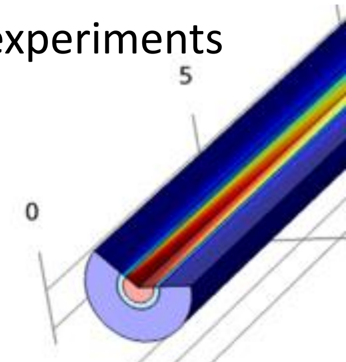
Cf Efrem course



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3 Post-Processing

Accurate representation of reality ?

3

Validation

Representation of the real world ?

Post-processing → Validation

Validation

- Computing accuracy ?

  - Change mesh to smaller size should not change the solution

  - Use the code for simple cases (having analytical solutions)
    - By changing the geometry
    - By changing the field equations
    - by changing initial/boundary conditions

- Accurate representation of real world ?

  - Compare the simulation results with available data

  - Realise sensitivity analysis (often based on dimensionless number) and parametric studies

CFD reliability

Water flow	Laminar	Turbulent	Transfer in blood or tissue
	No coupling	Momentum, Heat and Mass coupling	
	Incompressible Open Flow	Compressible Confined	
	Ideal phase	Non-ideal (interactions …)	
	Single phase	Mutiphasic with phase changes	
	Inert	Multiple chemical reaction	
	Strong reliability	Weak reliability	

CFD and biological applications

Taylor, C. A., Draney, M. T., Ku, J. P., Parker, D., Steele, B. N., Wang, K., & Zarins, C. K. (1999). Predictive medicine: computational techniques in therapeutic decision-making. *Computer aided surgery*, *4*(5), 231-247.

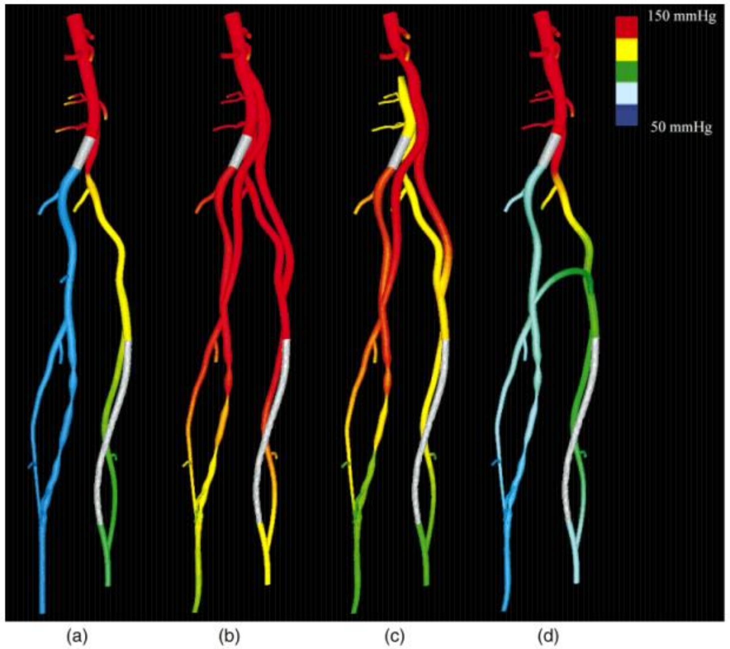


Fig. 8. Pressure distribution under resting conditions at peak systole for (a) pre-operative model, (b) aorto-femoral bypass graft with proximal end-to-side anastomosis, (c) aorto-femoral bypass graft with proximal end-to-end anastomosis, (d) balloon angioplasty in left common iliac artery with femoral-to-femoral bypass graft.

Blood flow

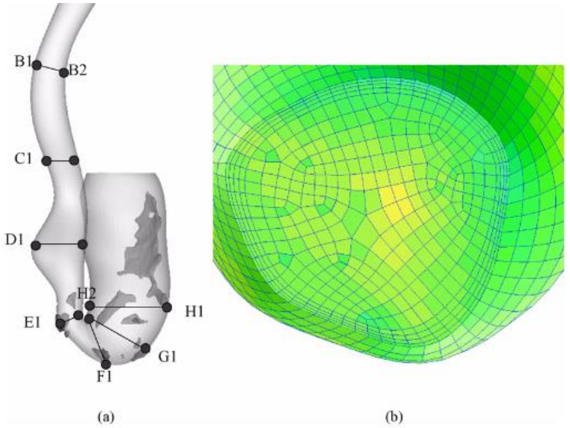
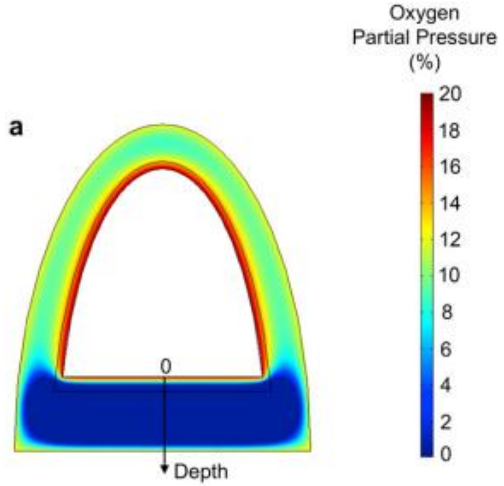


Fig. 1. (a) Representation of the volume of the AVF. This volume was divided into sevens sub-volumes. Six sub-sections and the location of their corresponding points under study. The black areas are the calcification plaques found on the vascular wall in the CT images. (b) Cross section meshed with hexahedral elements at plane F.

Kharboutly, Z., Fenech, M., Treutenaere, J. M., Claude, I., & Legallais, C. (2007). Investigations into the relationship between hemodynamics and vascular alterations in an established arteriovenous fistula. *Medical engineering & physics*, *29*(9), 999-1007.

Curcio, E., Macchiarini, P., & De Bartolo, L. (2010). Oxygen mass transfer in a human tissue-engineered trachea. *Biomaterials*, *31*(19), 5131-5136.



Oxygen transfer

CFD and biomedical applications

- Heart pumping and blood flows → cardiac valve design
- Air flow in lungs and gases exchanges → Oxygenator design
- Mechanical properties, lubrification → Prothesis design

- Transfer in tissue → Bioartificial organ design

CFD : a computer assisted by a human !

Engineering | Physics – Chemistry | Mathematics-Computation | Engineering

Real world → Conceptual model → PDE → Computer model → Post-processing → Validation

Provide acceptable level of complexity ?

Numerical recipes
(discretization techniques)
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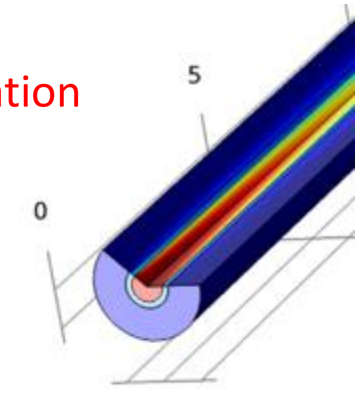
Accurate representation of reality ?



A lot of questions can not be answered by the computer until now !

Formulate the model
- What should be solved ?
- Assumptions, limiting phenomena ?

Define the problem
- Geometry, boundary conditions ?

Check the results
- Solution valid ?

Analyse the results
- Answer to initial questions ?