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UNIVERSITÀ DEGLI STUDI DI PALERMO

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CFD analysis of mass transfer in spacer-filled channels for reverse electrodialysis

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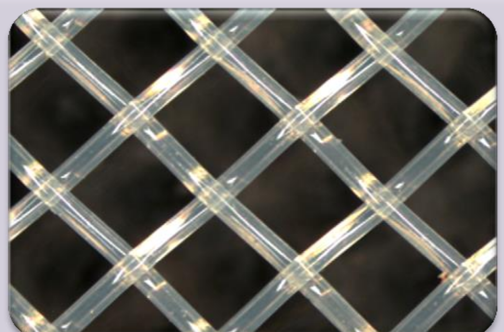
RED CHANNELS

Channel geometry → Fluid Dynamics → Performance

- Hydraulic friction
- Concentration Polarization

Net spacers for membranes separation



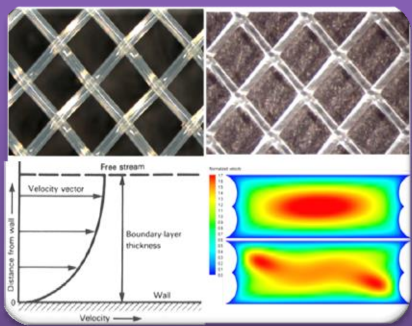
Two layers (overlapped) filaments

Woven filaments

✓ Mixing promotion

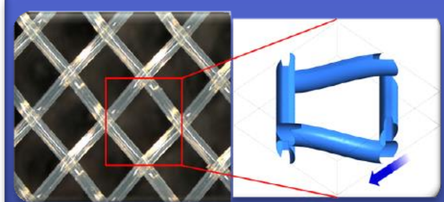
✠ Higher friction factor

OBJECTIVES, TOOLS AND ACTIVITIES

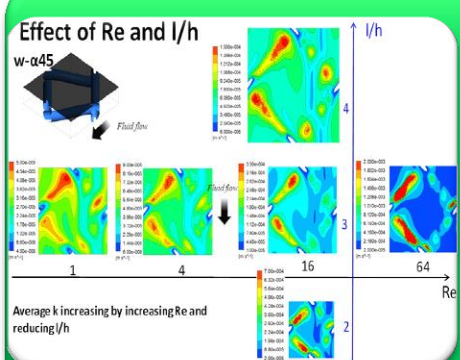


Objective: prediction of fluid flow and mass transfer in spacer-filled channels for RED applications

⇨ Process optimization



Tools: 3D-Computational Fluid Dynamics (CFD) modelling



Activities: parametric analysis

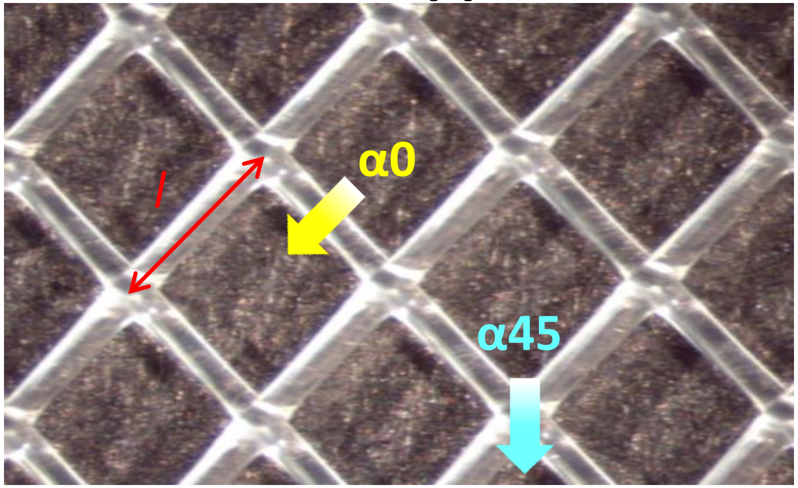
- Wires shape: woven and non woven spacers
- Pitch to height ratio (*l/h*)
- Channel orientation (fluid flow direction)
- Reynolds numbers typical of RED applications

NUMERICAL METHODOLOGIES

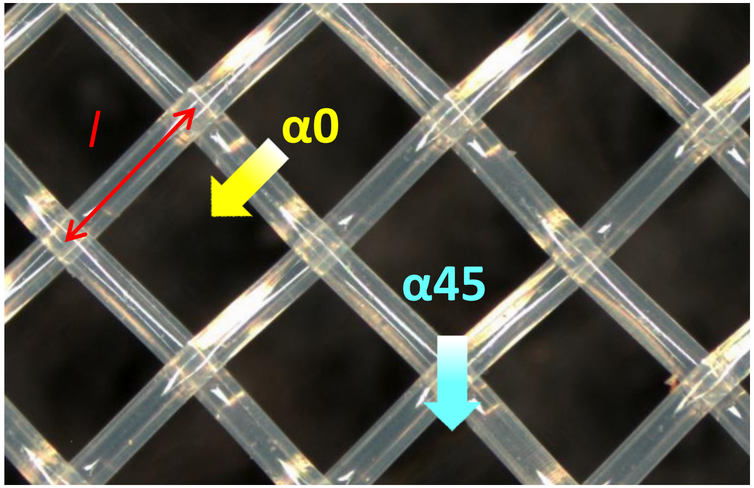
CASES INVESTIGATED

Diamond spacers

Overlapped



Woven



Filaments shape

- Overlapped (o)
- Woven (w)

Size

Pitch to height ratio l/h = 2, 3, 4
(h = 0.3 mm)

Fluid flow direction *α*

- 0°
- 45°

Reynolds number *Re*

1, 4, 16, 64

CFD MODELING

The finite volumes code **Ansys-CFX 14** was employed to discretize and solve the governing equations (Newtonian and incompressible fluid). **Steady** regime at all flow rates investigated

$$\vec{\nabla}\cdot\vec{u}=0$$

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho\vec{u}\vec{\nabla}\cdot\vec{u}=-\vec{\nabla}p+\mu\nabla^{2}\vec{u}+\vec{P}$$

Body force → fluid motion in a periodic domain

$$\vec{\nabla}\left(\tilde{C}\vec{u}\right)=\vec{\nabla}\left[D\frac{b}{b+\left(a-M_{e}\right)\left(\tilde{C}+ks\right)}\vec{\nabla}\tilde{C}\right]-ku_{s}$$

NaCl solution at T = 25 °C	Molarity [mol/l]	Density [kg/m³]	Viscosity [Pa s]	Diffusivity [m²/s]
Seawater	0.5	1017.2	9.31e-04	1.47e-09

For details see *L. Gurreri, A. Tamburini, A. Cipollina, G. Micale, M. Ciofalo, CFD prediction of concentration polarization phenomena in spacer-filled channels for reverse electrodialysis, J. Membr. Sci., 468 (2014) 133-148.*

BASIC EQUATIONS*

Transport equation for a binary electrolyte

Multicomponent diffusion equation (Stefan-Maxwell)

$$C_i \overline{\nabla} \mu_i = \sum_j K_{ij} \left(\overline{u_j} - \overline{u_i} \right) = RT \sum_j \frac{C_i C_j}{C_T D_{ij}} \left(\overline{u_j} - \overline{u_i} \right)$$

Electroneutrality condition binary electrolyte

$$z_+ C_+ = -z_- C_-$$

solvent velocity ≈ *u*

salt diffusivity

solvent concentration

transport number

$$\underbrace{\frac{\partial C}{\partial t}}_{\text{Accumulation}} + \underbrace{\overline{\nabla}\left(C \overline{u}_0 \right)}_{\text{Convection}} = \underbrace{\overline{\nabla} \cdot \left[D \left(1 - \frac{d \ln C_0}{d \ln C} \right) \overline{\nabla} C \right]}_{\text{Diffusion}} \underbrace{- \frac{\overline{i} \cdot \overline{\nabla} t_i^0}{z_i \nu_i F}}_{\text{Migration}}$$

J.S. Newman, Electrochemical Systems, Second Edition, 2nd edition, Prentice Hall, Englewood Cliffs, NJ (1991)

K. Kontturi, L Murtomäki, J.A. Manzanares, Ionic Transport Processes In Electrochemistry and Membrane Science, Oxford University Press (2008)

CFD MODELLING DEVELOPMENT

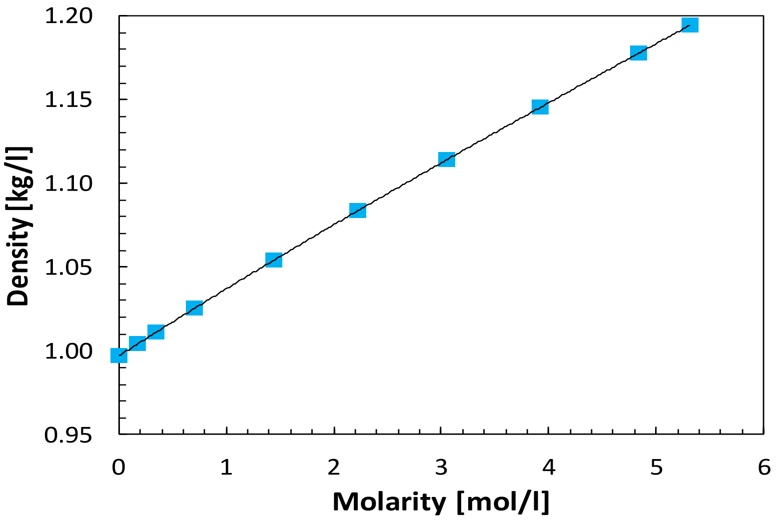
Implementation of transport equations

Assuming density as a linear function of *C*

$$\rho = aC + b$$

Diffusive term

$$\left(1 - \frac{d\ln C_0}{d\ln C}\right) = \frac{\rho - C\dfrac{d\rho}{dC}}{C_0 M_0} = \frac{b}{b + \left(a - M_C\right)C}$$



CFD MODELLING DEVELOPMENT

Implementation of transport equations

Migrative term

$$\frac{\partial C}{\partial t}+\overline{\nabla}\left(C\overline{u}_0\right)=\overline{\nabla}\cdot\left[D\frac{b}{b+\left(a-M_C\right)C}\overline{\nabla}C\right]-\frac{\overline{i}\cdot\overline{\nabla}t_i^0}{z_i\nu_i F}$$

- Current density
- Equations system not closed
- Above transport equation can be solved
  - when coupled with other equations → entire stack as domain
  - or when current density distribution is known (spacer-less channel)

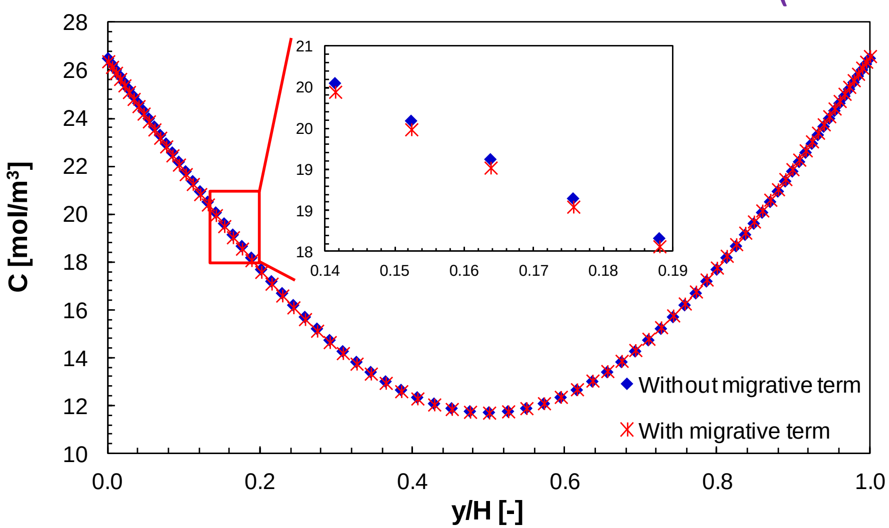
CFD MODELLING DEVELOPMENT

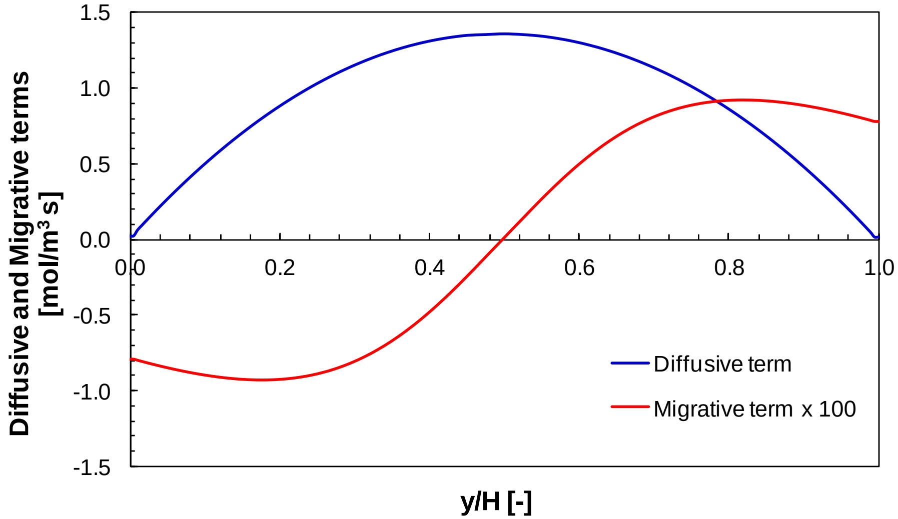
Implementation of transport equations

Simulations of an empty channel

- Concentration profiles were unaffected by the migrative term
- Migrative term is negligible compared to the diffusive one
- → Migrative flux is quite uniform

most unfavourable case (low concentration and high current density)





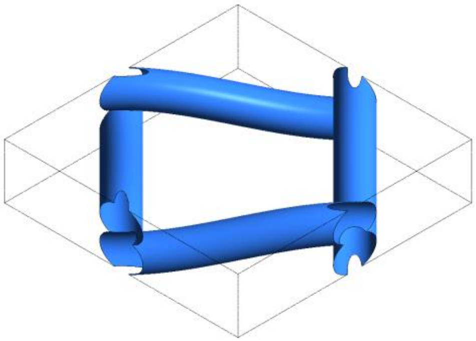
$$\frac{\partial C}{\partial t}+\bar{\nabla}\left(C\bar{u}_0\right)=\bar{\nabla}\cdot\left[D\frac{b}{b+\left(a-M_C\right)C}\bar{\nabla}C\right]\cancel{-\frac{\bar{i}\cdot\bar{\nabla}t_i^0}{z_i\nu_i F}}$$

Migrative term neglected

MODELLING APPROACH

Transport equation implemented for Unit Cell

Fully developed flow → Linear variation of concentration along the flow direction (s)
Periodic boundary conditions despite the change of the bulk concentration



$$C = \tilde{C}(x, y, z, t) + k \cdot s$$

Periodic concentration

Conc. gradient

Fluid flow direction

Transport equation for the electrolyte in unit cell

$$\frac{\partial \tilde{C}}{\partial t} + \vec{\nabla}\left(\tilde{C}\vec{u}\right) = \vec{\nabla}\left[D\frac{b}{b+\left(a-M_e\right)\left(\tilde{C}+ks\right)}\vec{\nabla}\tilde{C}\right] - ku_s$$

$$k = \frac{Q_{TOT}}{V \cdot u_{s,ave}}$$

$$Q_{TOT} = J \cdot (A_{CEM} + A_{AEM})$$

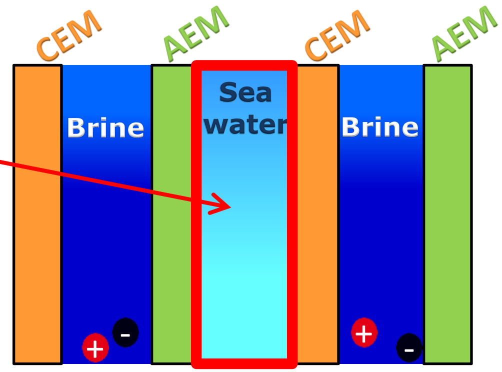
Ingoing flux throug membrane

MODELLING APPROACH

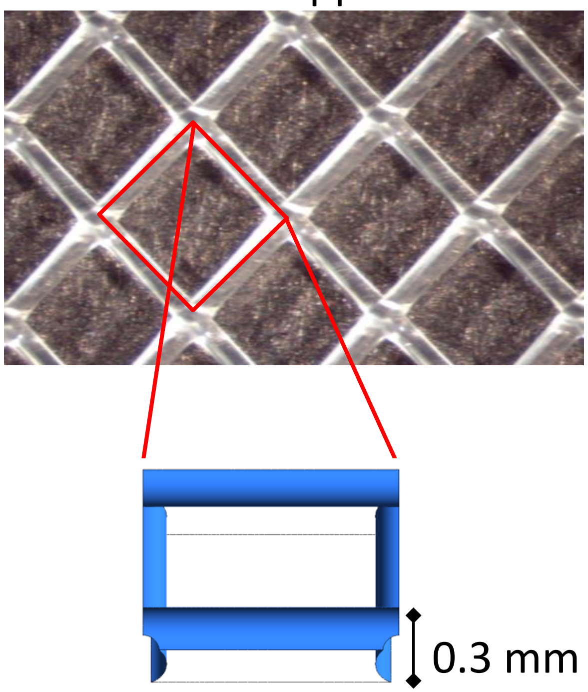
Computational domain

One channel

No double layer

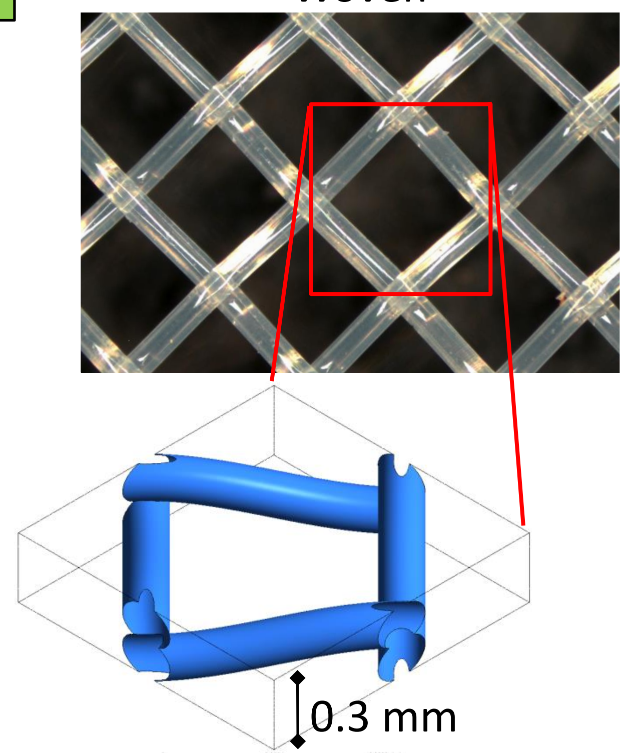


Overlapped



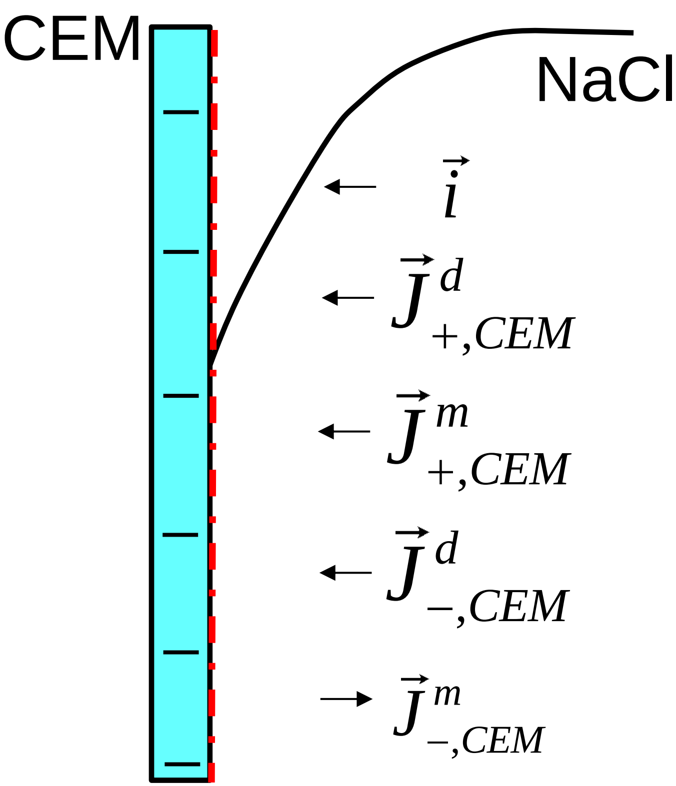
Unit Cell

Woven



MODELLING APPROACH

Wall boundary at membrane-solution interface



$$\vec{J}_i^{m} = \frac{t_i^0}{z_i F}\vec{i}$$

$$\alpha = 1 \quad \Rightarrow \quad \vec{J}^{tot}_{-,CEM} = 0 = \vec{J}^{d}_{-,CEM} + \vec{J}^{m}_{-,CEM}$$

$$\vec{J}^{d}_{-,CEM} = -\vec{J}^{m}_{-,CEM} = -\frac{t_-^0}{z_- F}\vec{i}$$

$$\vec{J}^{d}_{CEM} = \frac{\vec{J}^{d}_{-,CEM}}{\nu_-} = -\frac{t_-^0}{\nu_- z_- F}\vec{i} \approx \frac{0.5}{F}\vec{i}$$

Uniform flux at the **membrane-solution interfaces**

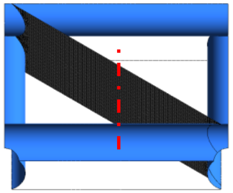
MODELLING APPROACH

Mesh and *grid dependence analysis*

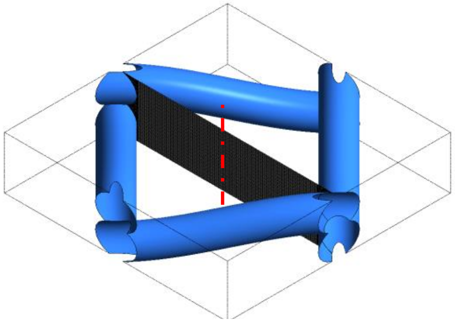
Grid dependence by varying the size
- results independent of the discretization degree
- accuracy
- computational savings

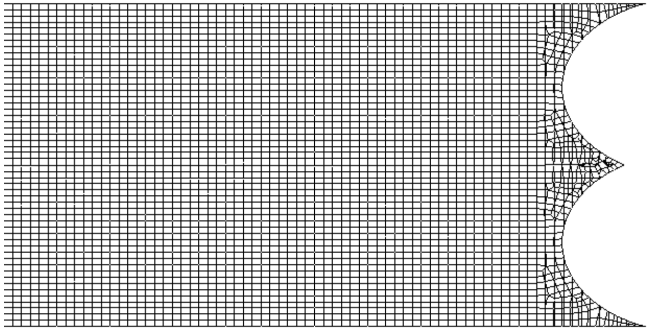
Size = 0.006 mm
420,000 - 5,760,000 vol.

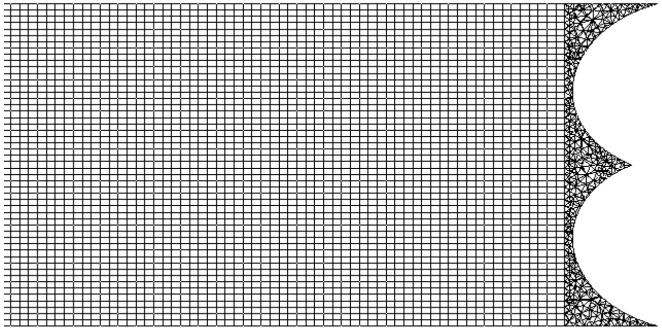
Overlapped



Woven





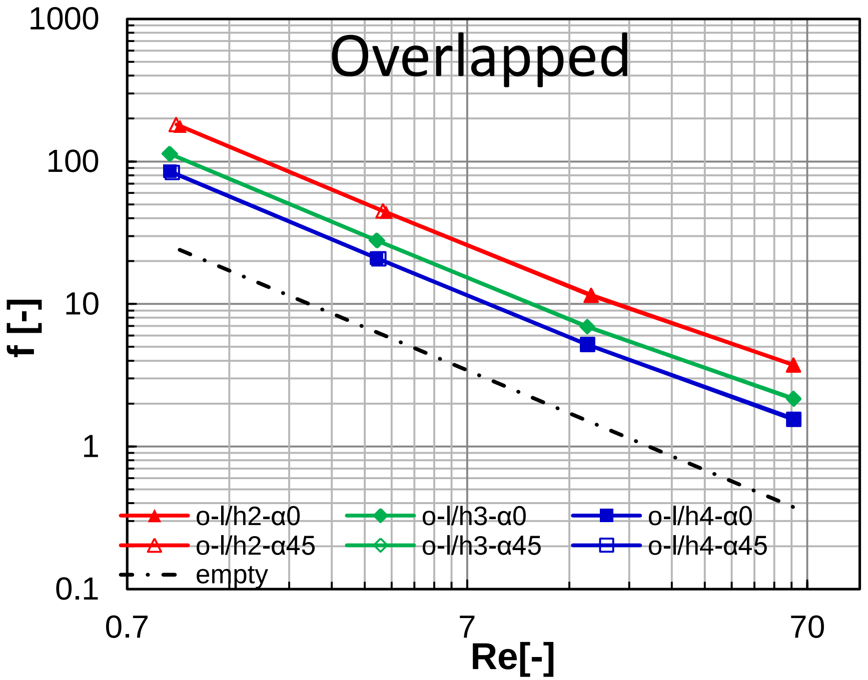


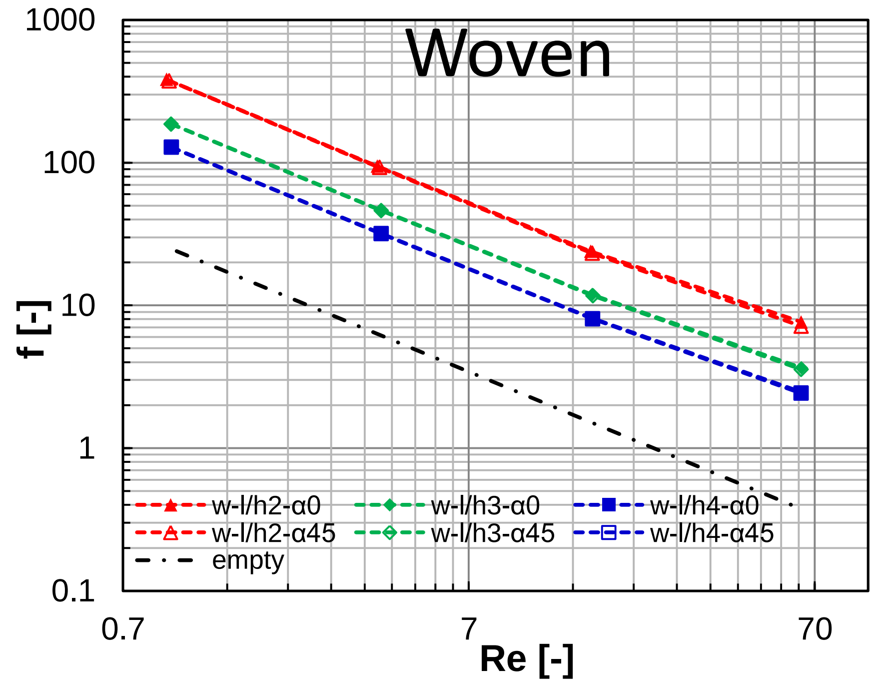
RESULTS

Pressure drop

FRICTION FACTOR

$$f = \frac{\Delta p}{l}\frac{d_h}{2\rho u_{s,mean}^2} \qquad f = ARe^n$$





•The presence of obstacles causes ***f* higher than the empty ch**.

• ***α*** has irrelevant effects

• *f* reduces by increasing the **pitch**

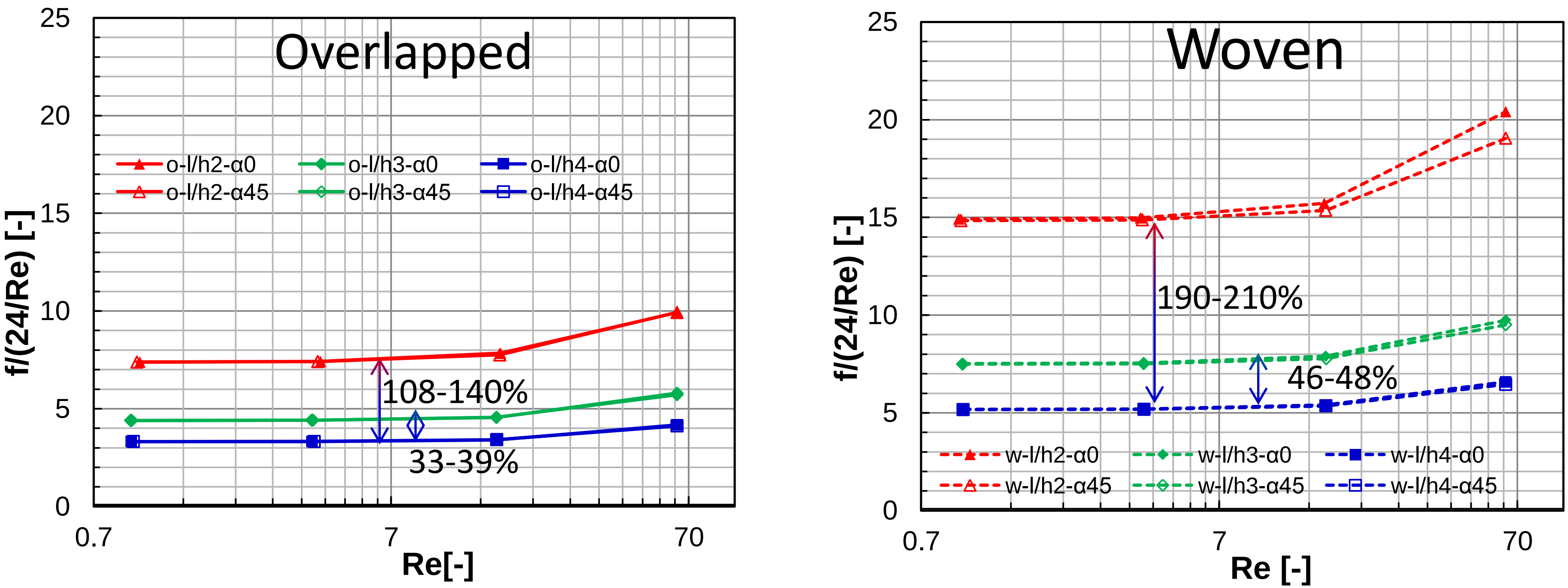
• W-**shape** implies *f* higher than the o

• At the lowest Re numbers, *n = -1* → creeping flow

• At higher Re, *n* deviates from -1, since the obstacles induce increasing inertial effects → flow fields not self-similar

PRESSURE DROP NORMALIZED

$$f_{empty} = 24Re^{-1}$$



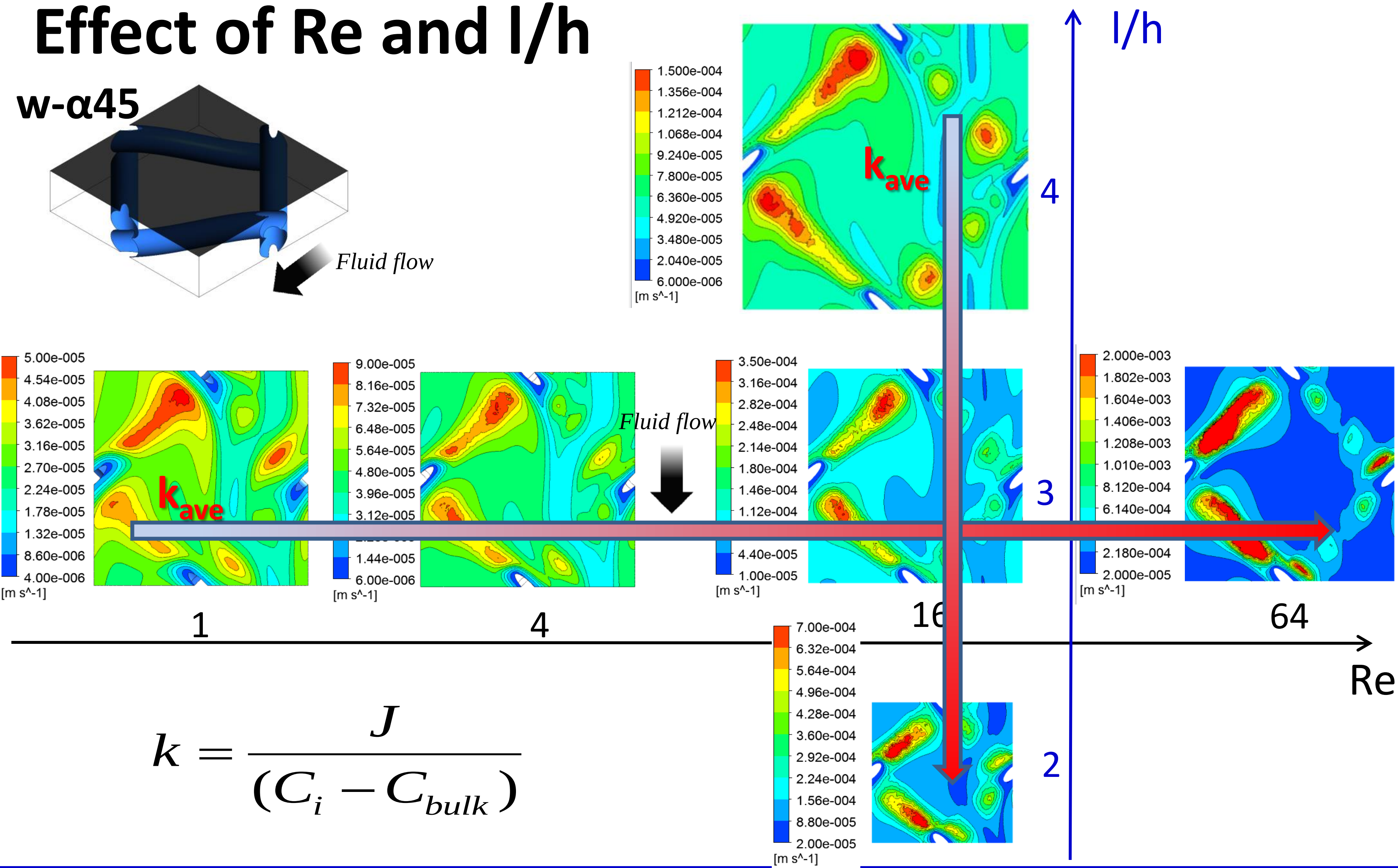
- **Spacers** provide *f* **3-20 times** higher than the **empty ch**.
- ***α*** is **irrelevant** at these Re

- The **pitch** has significant effects, especially for the w-shape
- **W-shape** leads to **pressure drop increase** by 106%, 67%, 54%, for l/h=2,3,4 respectively

Mass transfer

MASS TRANSFER COEFFICIENT

Effect of Re and l/h

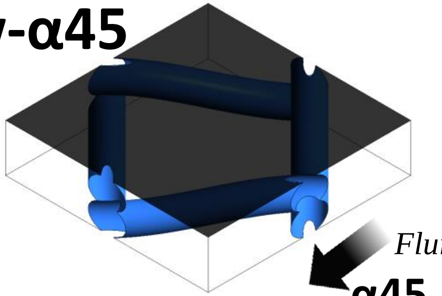


$$k = \frac{J}{(C_i - C_{bulk})}$$

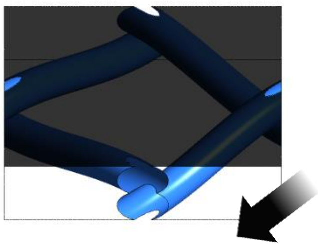
MASS TRANSFER COEFFICIENT

Effect of α in w-shape

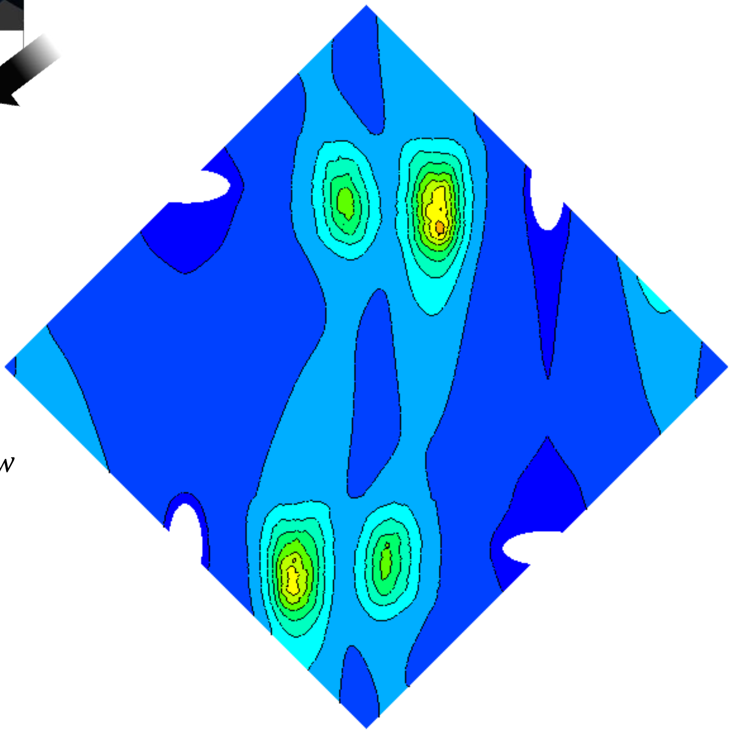
w-α45



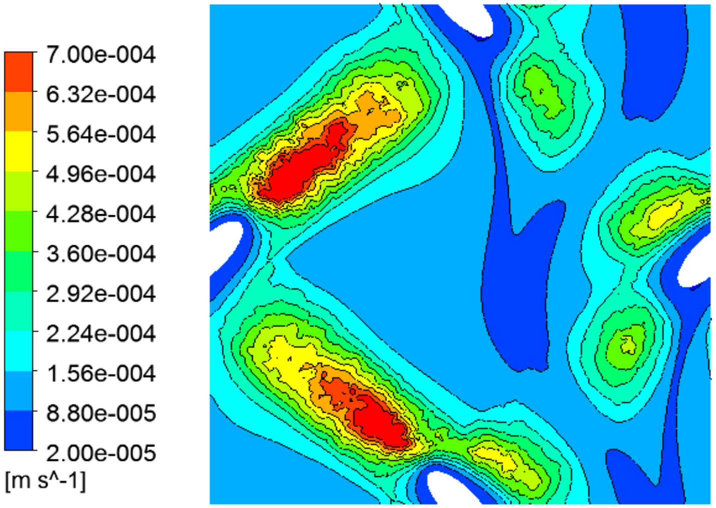
w-α0



w-l/h2-α0



w-l/h2-α45



Fluid flow

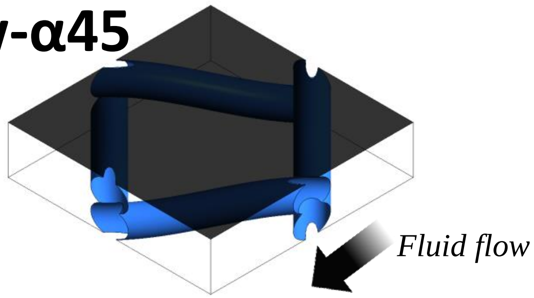
Re=16

$k_{w\text{-}\alpha 45} > k_{w\text{-}\alpha 0}$

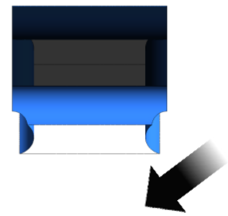
MASS TRANSFER COEFFICIENT

Effect of filaments shape

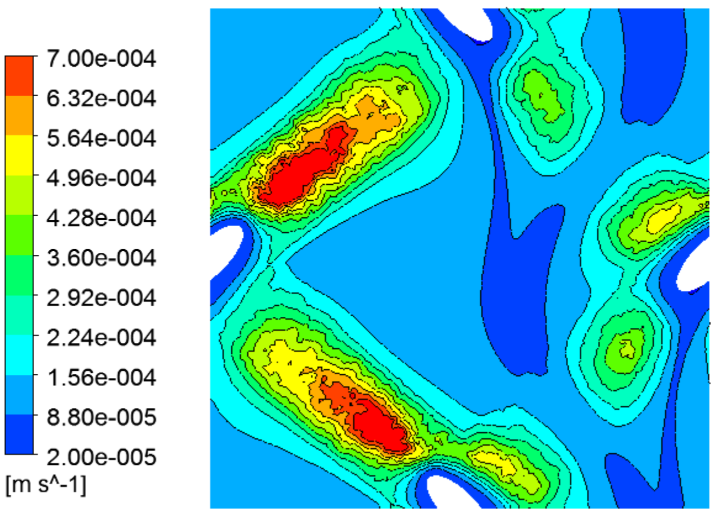
w-α45



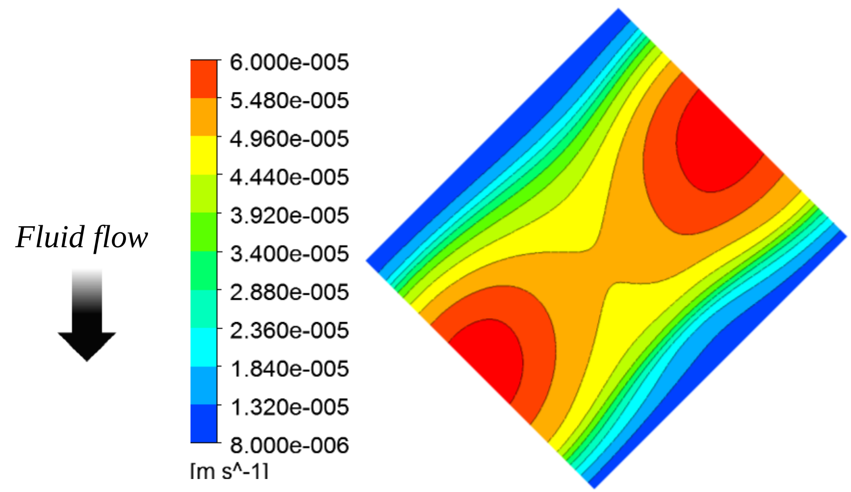
o-α45



w-l/h2-α45



o-l/h2-α45



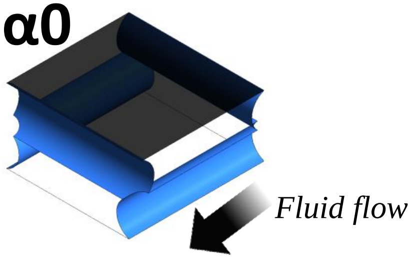
Re=16

$k_w > k_o$

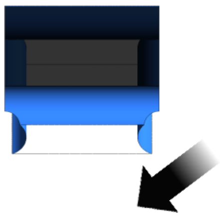
MASS TRANSFER COEFFICIENT

Effect of α in o-shape

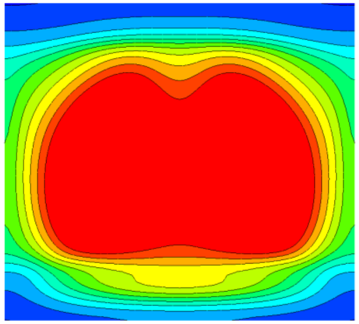
o-α0

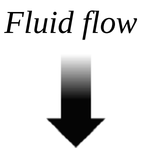


o-α45

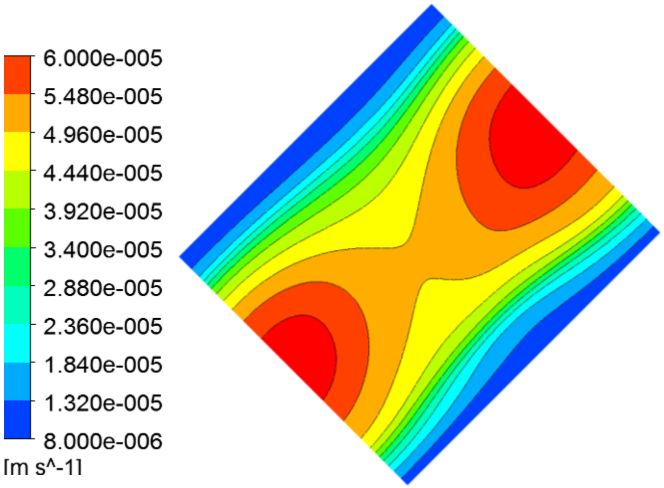


o-l/h2-α0





o-l/h2-α45



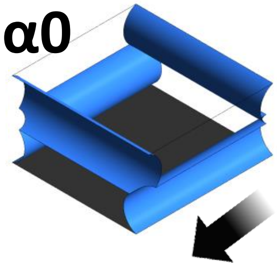
Re=16

Different distribution, but similar k_{ave}

MASS TRANSFER COEFFICIENT

Effect of α in o-shape

o-α0

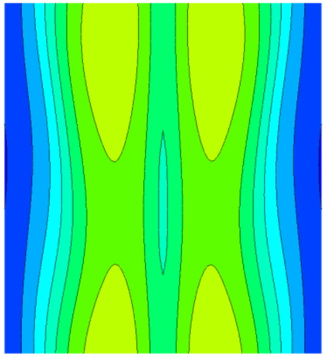


o-α45

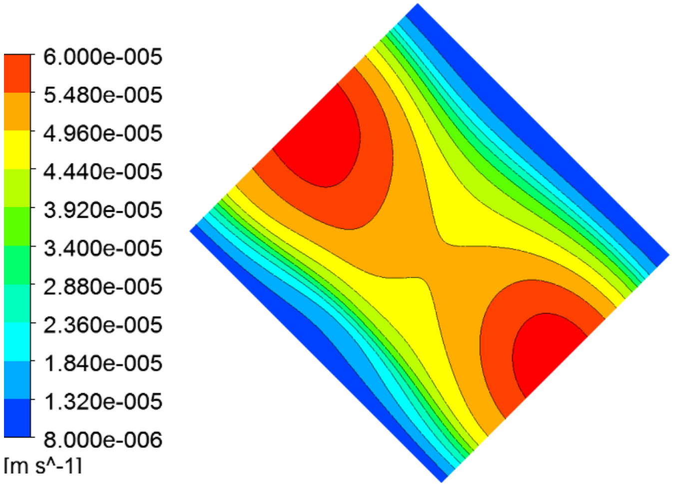
o-l/h2-α45

Significant effect of the asymmetry for o-α0

o-l/h2-α0



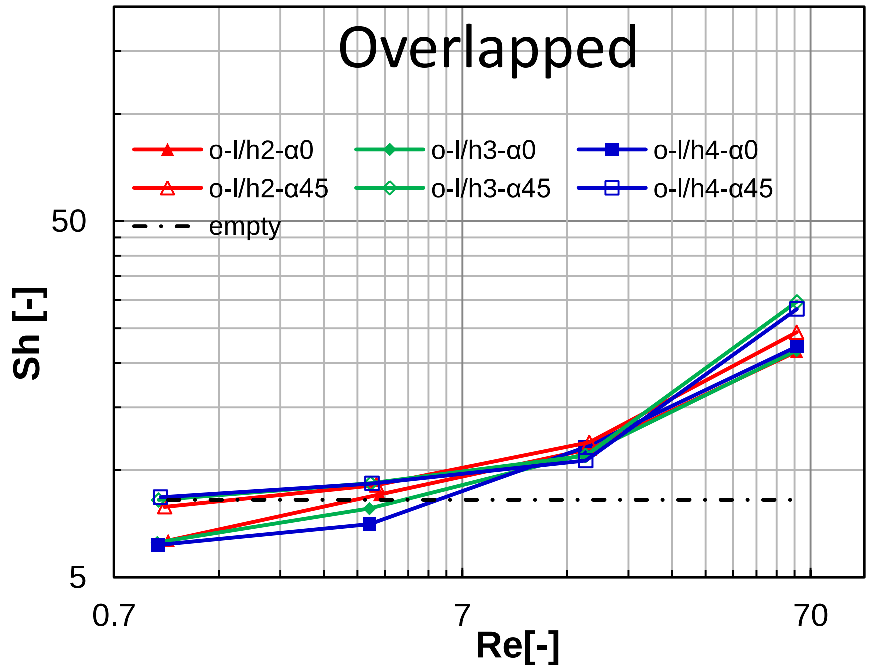
Fluid flow

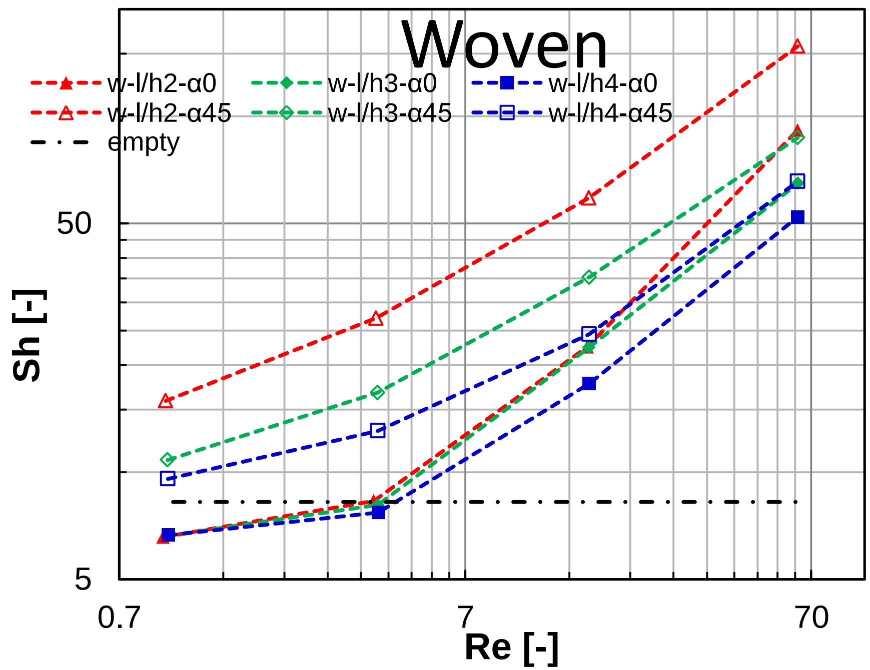


Re=16

SHERWOOD NUMBER

$$Sh = \frac{k\, d_h}{D}$$





• **Mixing not favored at very low Re** due to the calm regions caused by the filaments, especially for α0. **Sh much higher** at higher Re

• $\boldsymbol{Sh_{w\text{-}\alpha45}}$ **reduces by increasing l/h**, for α0 this occurs only at the highest Re; for o-shape the dependence on l/h is not significant

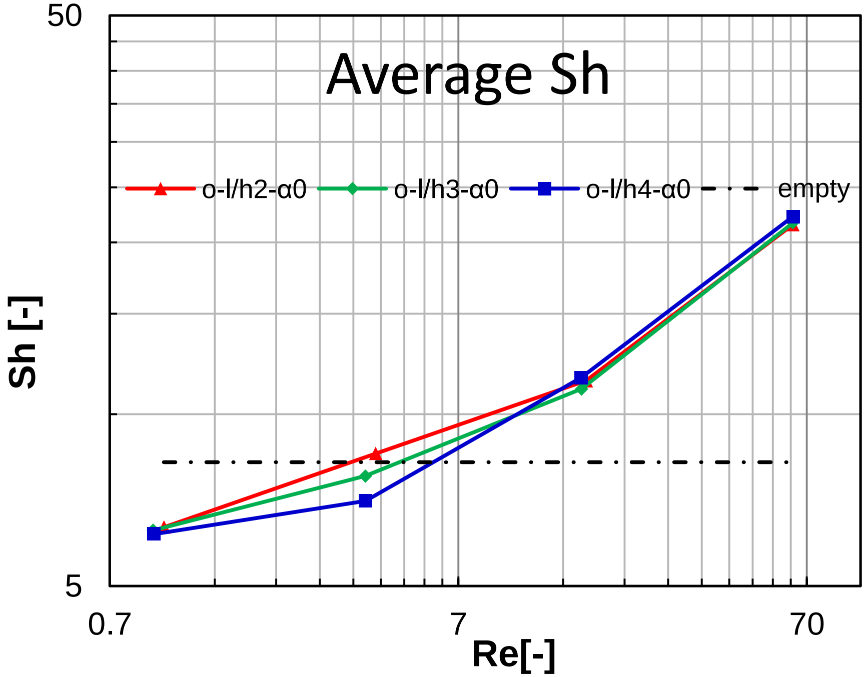
• *α*: $\boldsymbol{Sh_{w\text{-}\alpha45} > Sh_{w\text{-}\alpha0}}$; for o-shape the effect is slighter, but the influence of Re is more complex

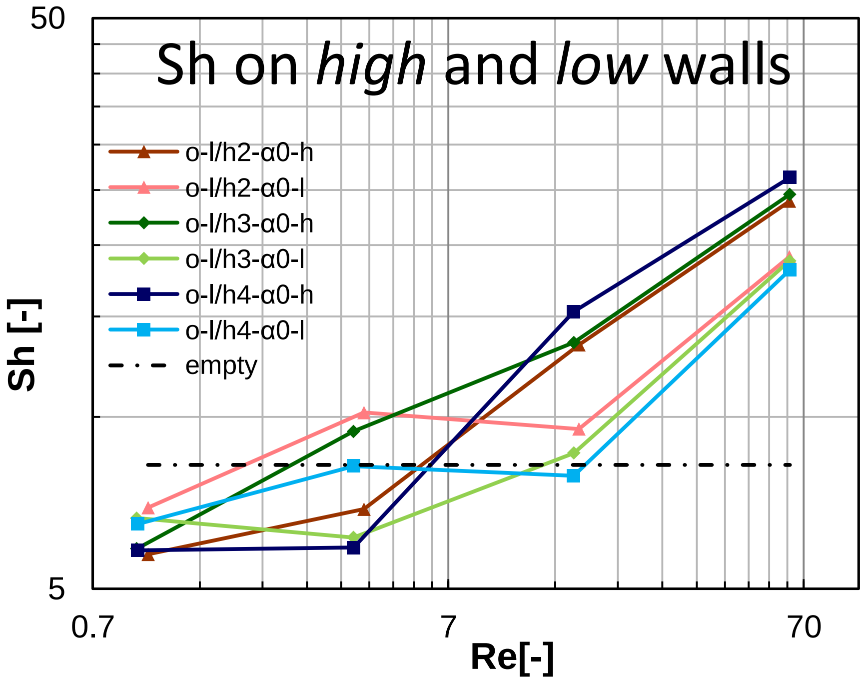
• $\boldsymbol{Sh_w > Sh_o}$

SHERWOOD NUMBER

$$Sh = \frac{k\, d_h}{D}$$

Overlapped-α0



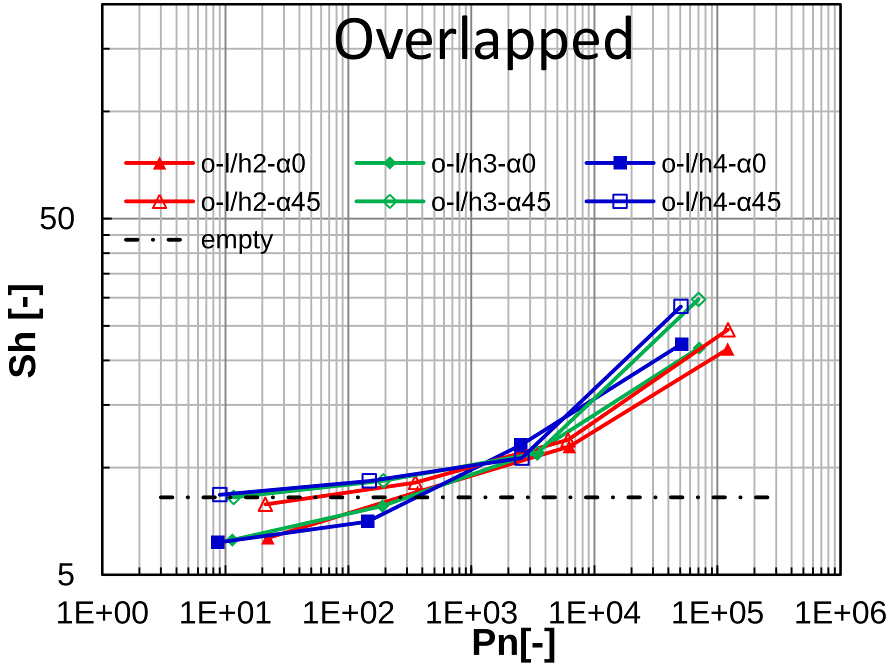


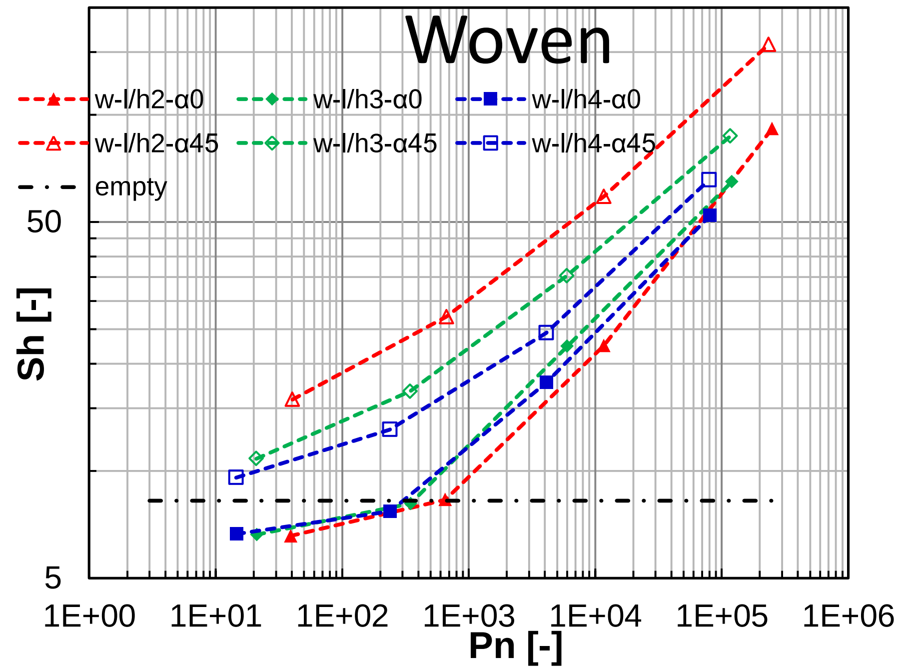
- **Overlapped-α0** is the only case with **asymmetry** → distribution and average Sh different at the two walls
- Very different behavior for the *high* and the *low* walls
- Trend not straightforward with Re

SHERWOOD NUMBER

$$Sh = \frac{k\, d_h}{D}$$

Power number $$Pn = \mathrm{SPC}\frac{\rho^2 h^4}{\mu^3} = \frac{1}{8} f\, Re^3 \qquad \mathrm{SPC} = \frac{\Delta p}{l} u_{s,mean}$$





• ***Pn***: dimensionless pumping power consumption

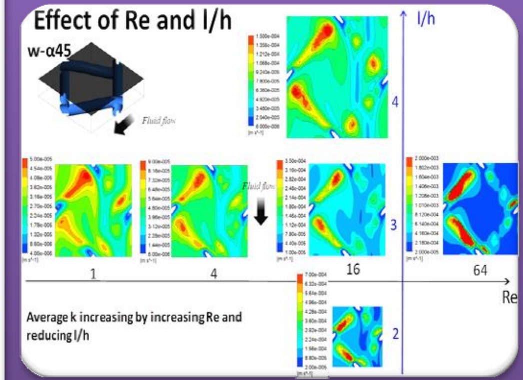
• In a quantitative analysis, the trends of Sh=f(Pn) are different with respect to Sh=f(Re)

• Qualitatively, the same considerations can be applied as before

•As a difference, the pitch has not a significant effect for the w-α0

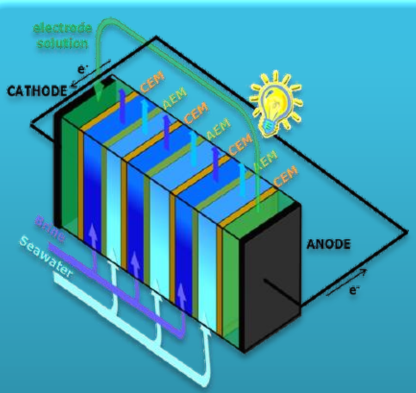
CONCLUSIONS

CONCLUSIONS



CFD modelling of spacer filled ch. for RED

- Fluid flow and mass transfer behaviour
- Parametric analysis of:
  - Wires shape: woven and non woven spacers
  - Pitch to height ratio (*l/h*)
  - Channel orientation (fluid flow direction)
  - Re effects
- Process efficiency: Pn and Sh



OPTIMAL CHANNEL CONFIGURATION

Influence of various factors on efficiency.

Simulation results as input data for a process simulator

→ Optimal channel configuration and Re

Thank you for your attention

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