Numerical Analysis of Mass Transfer to the Anode in a Microbial Fuel Cell

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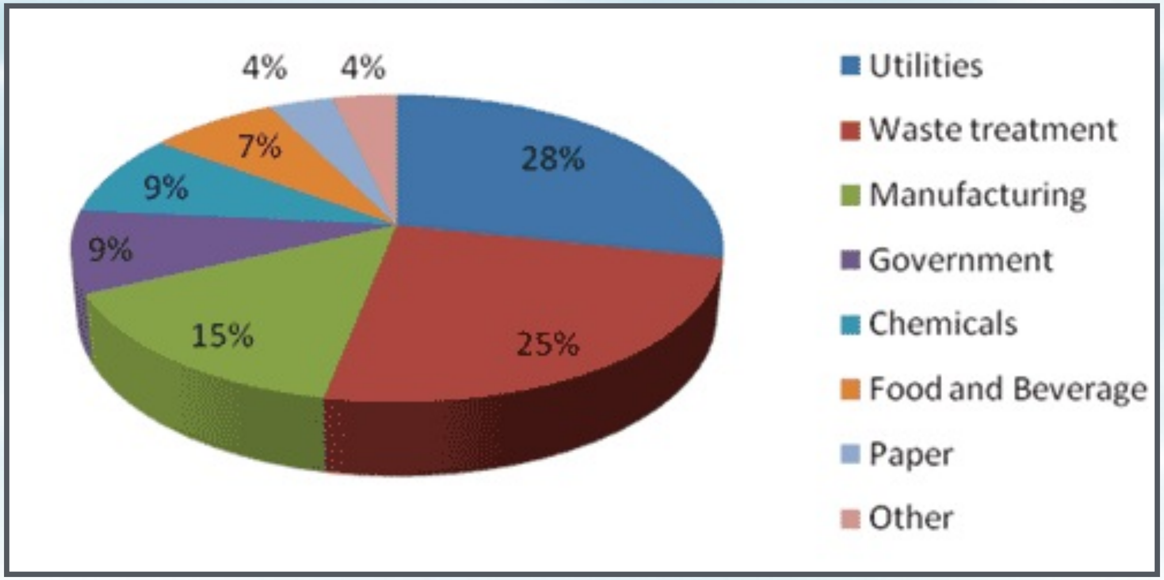
Agenda

- Introduction
- About Microbial Fuel Cells
- Mathematical Model
- Results of the Simulations
- Conclusion

Introduction - 1

- **High operating costs of wastewater treatment plants**
- **Transition from major energy consumers to energy neutrality or even net producers?**



Expenses of industrial facilities
Survey Industrial WaterWorld Magazine, 2010

Introduction - 2

- Microbial Fuel Cells (MFCs) are one possible technology for sustainable treatment
- Especially promising for selected industrial wastewater (Bierbaum, 2014), where other waste-to-energy technologies are not viable
- One milestone towards upscaling MFC: functional bioanode

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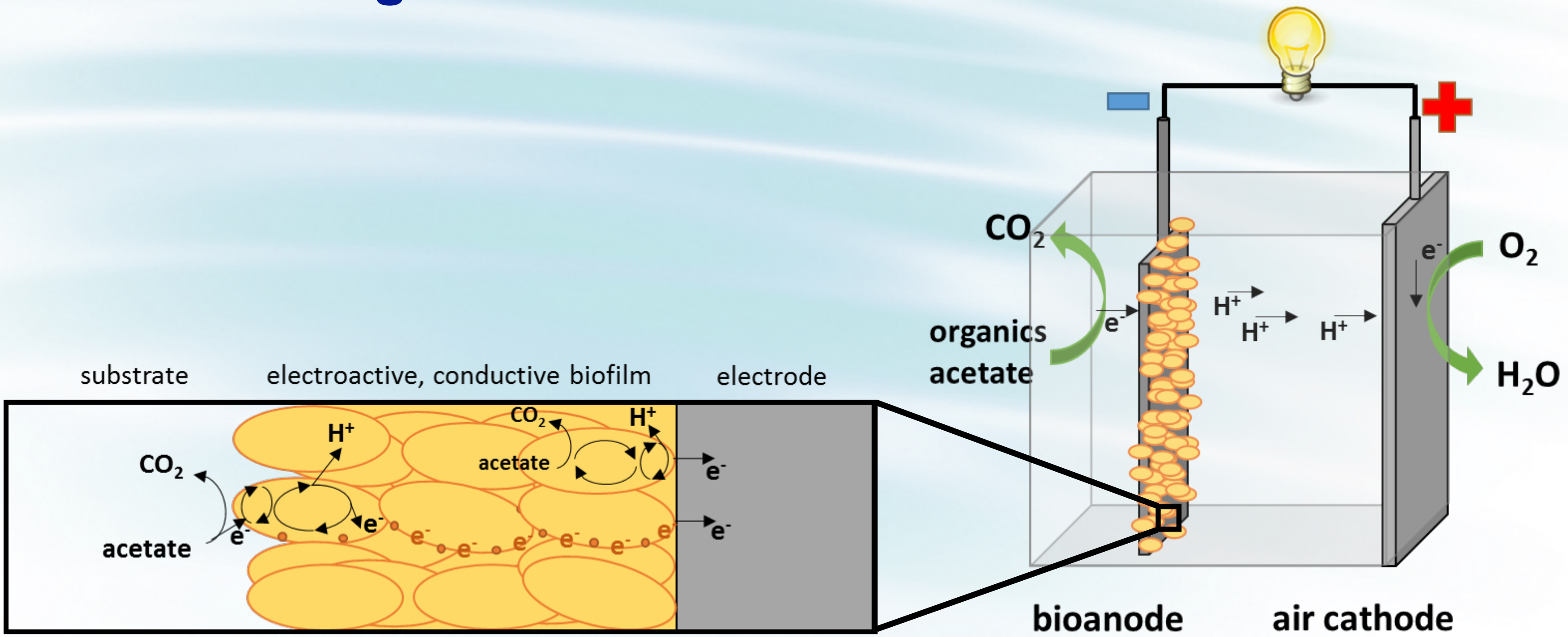
Microbial Fuel Cells - 1

- Electroactive bacteria generate electric current from organic substrates like acetate
- Model organism *Geobacter sulfurreducens* transfers electrons from substrate oxidation to electrode surface through a conductive biofilm matrix



Microbial Fuel Cells - 2

- **Sum redox reaction of an MFC with electro active model organism *Geobacter sulfurreducens:***

$$acetate + 2O_2 + H^+ \rightarrow 2CO_2 + 2H_2O$$

- **Splitting into half reactions allows energy harvest as electrons flow from low potential anode to high potential cathode**

- **For bioanode studies, a potentiostat fixes a defined potential at the anode (eleminates possible limitations by non-ideal cathode)**

bioanode:
- oxidation of substrate
- electron release

$$acetate + 2\ H_2O + H^+ \rightarrow 2\ CO_2 + 8\ e^- + 8\ H^+$$

air cathode:
- reduction of oxygen
- electron consumption

$$2\ O_2 + 8\ H^+ + 8\ e^- \rightarrow 4\ H_2O$$

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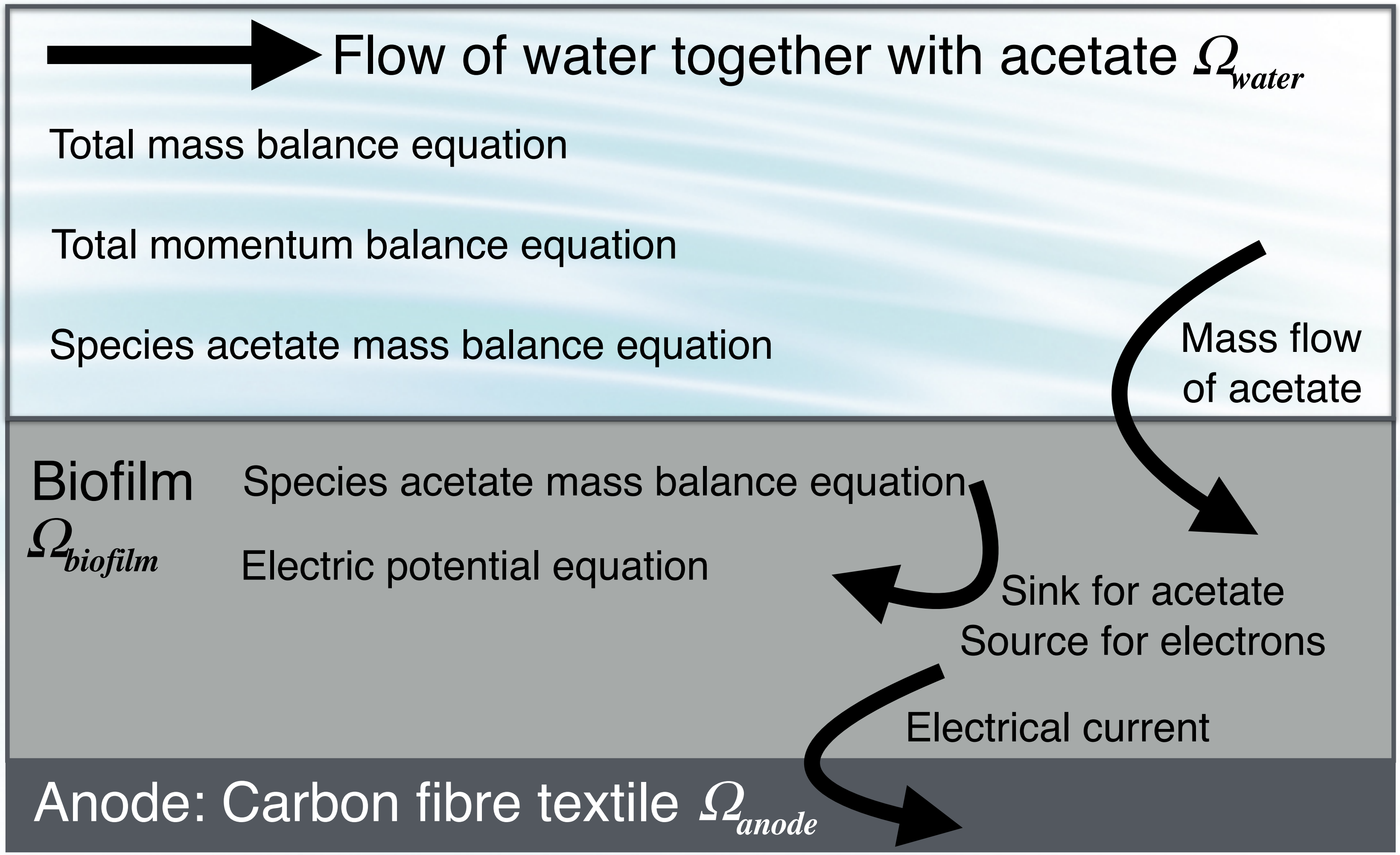
Mathematical Model - 1

- **Balance equations - 1: The mathematical model is an extension of the model of Merkey and Chopp (2012)**



Mathematical Model - 2

- **Balance equations - 2**

→ Flow of water together with acetate Ω_{water}

$$\nabla\cdot(\rho_1 \mathbf{v}) = 0 \qquad \rho_1 = \frac{1}{\frac{Y_{a,1}}{\rho_{a,1}} + \frac{Y_{w,1}}{\rho_{w,1}}}$$

$$\nabla\cdot(\rho_1 \mathbf{v}\otimes\mathbf{v}) = -\nabla p + \nabla\cdot\mathbf{T} \qquad \mathbf{T} = \mu_1\left[(\nabla\otimes\mathbf{v}) + (\nabla\otimes\mathbf{v})^{\mathrm{T}} - \frac{2}{3}\nabla\cdot\mathbf{v}\mathbf{I}\right] \qquad \boldsymbol{I} = \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$$

$$\nabla\cdot(\rho_1 \mathbf{v} Y_{a,1}) = \nabla\cdot(\rho_1 D_{a,1} \nabla Y_{a,1}) \qquad Y_{w,1} = 1 - Y_{a,1}$$

ρ_1 Density of the water/acetate mixture

$Y_{a,1}$ Mass fraction of acetate in Ω_{water}

$Y_{w,1}$ Mass fraction of water in Ω_{water}

μ_1 Viscosity of the water/acetate mixture

$D_{a,1}$ Diffusion coefficient of acetate in water

$\mathbf{v}$ Velocity vector

$\rho_{a,1}$ Density of acetate in Ω_{water}

$\rho_{w,1}$ Density of water in Ω_{water}

p Pressure

Mathematical Model - 3

- **Balance equations - 3**

ρ_2	Density of the biomass/acetate mixture	F	Faradays constant
$Y_{a,2}$	Mass fraction of acetate in $\Omega_{biofilm}$	R	Gas constant
$Y_{b,2}$	Mass fraction of biomass in $\Omega_{biofilm}$	T_2	Absolut temperature of biofilm
$Y_{a,1/2\max}$	Half-max rate of biomass	ϕ	Electric potential
C	Data fitting constant	λ	Acetate to electric current conversion
κ_{bio}	Electrical conductivity of the biofilm		

Biofilm $\Omega_{biofilm}$

$$0 = \nabla \cdot (\rho_2 D_{a,2} \nabla Y_{a,2}) - C \frac{Y_{a,2}}{Y_{a,1/2\max} + Y_{a,2}} \frac{1}{1 + e^{-\frac{F}{RT_2}\phi}}$$

$$Y_{b,2} = 1 - Y_{a,2}$$

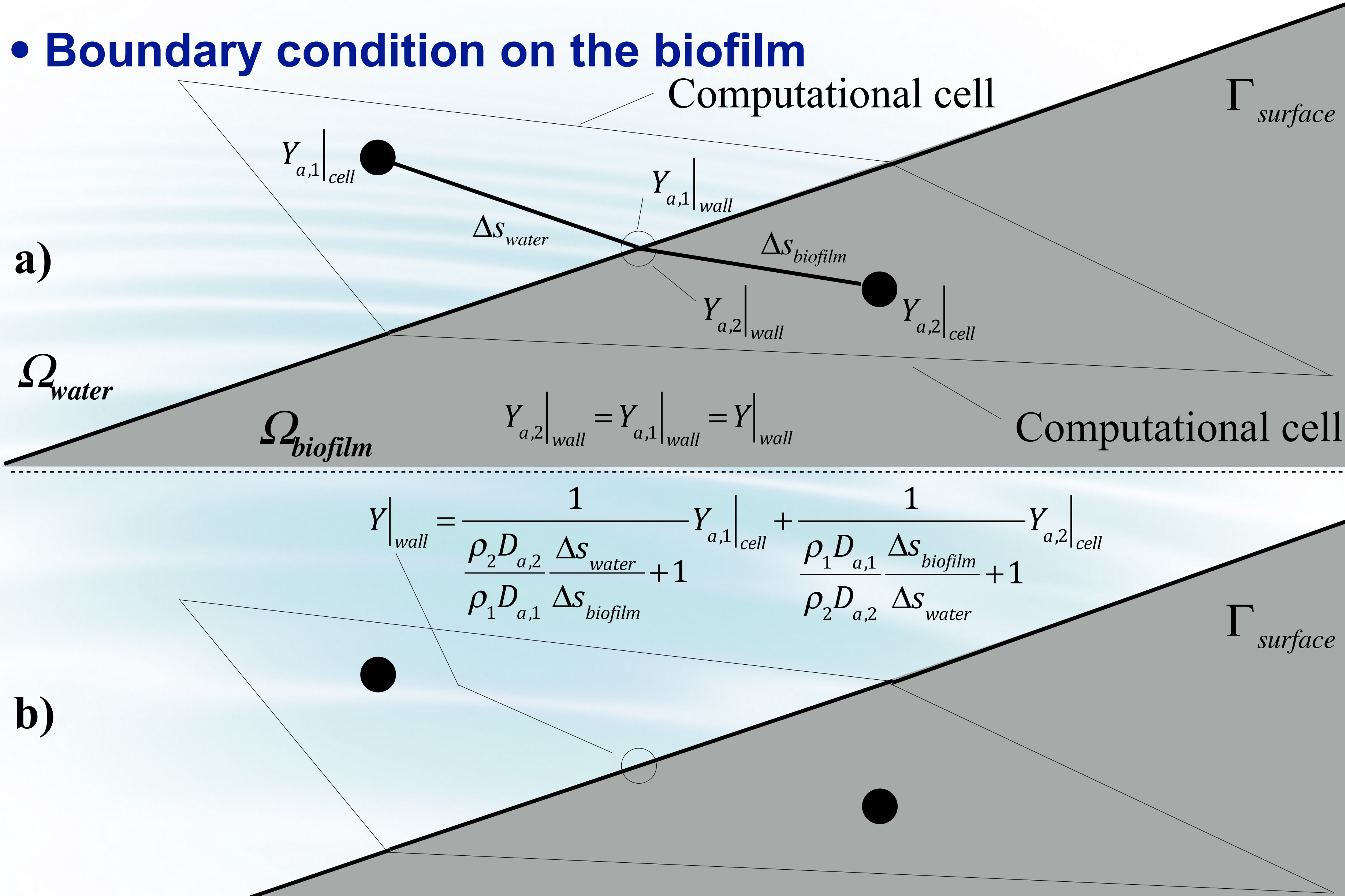
$$0 = \nabla \cdot (\kappa_{bio} \nabla \phi) - \lambda C \frac{Y_{a,2}}{Y_{a,1/2\max} + Y_{a,2}} \frac{1}{1 + e^{-\frac{F}{RT_2}\phi}}$$

$$\rho_2 = \frac{1}{\frac{Y_{a,2}}{\rho_{a,2}} + \frac{Y_{b,2}}{\rho_{b,2}}}$$

Anode: Carbon fibre textile Ω_{anode}

Mathematical Model - 4

- **Boundary condition on the biofilm**

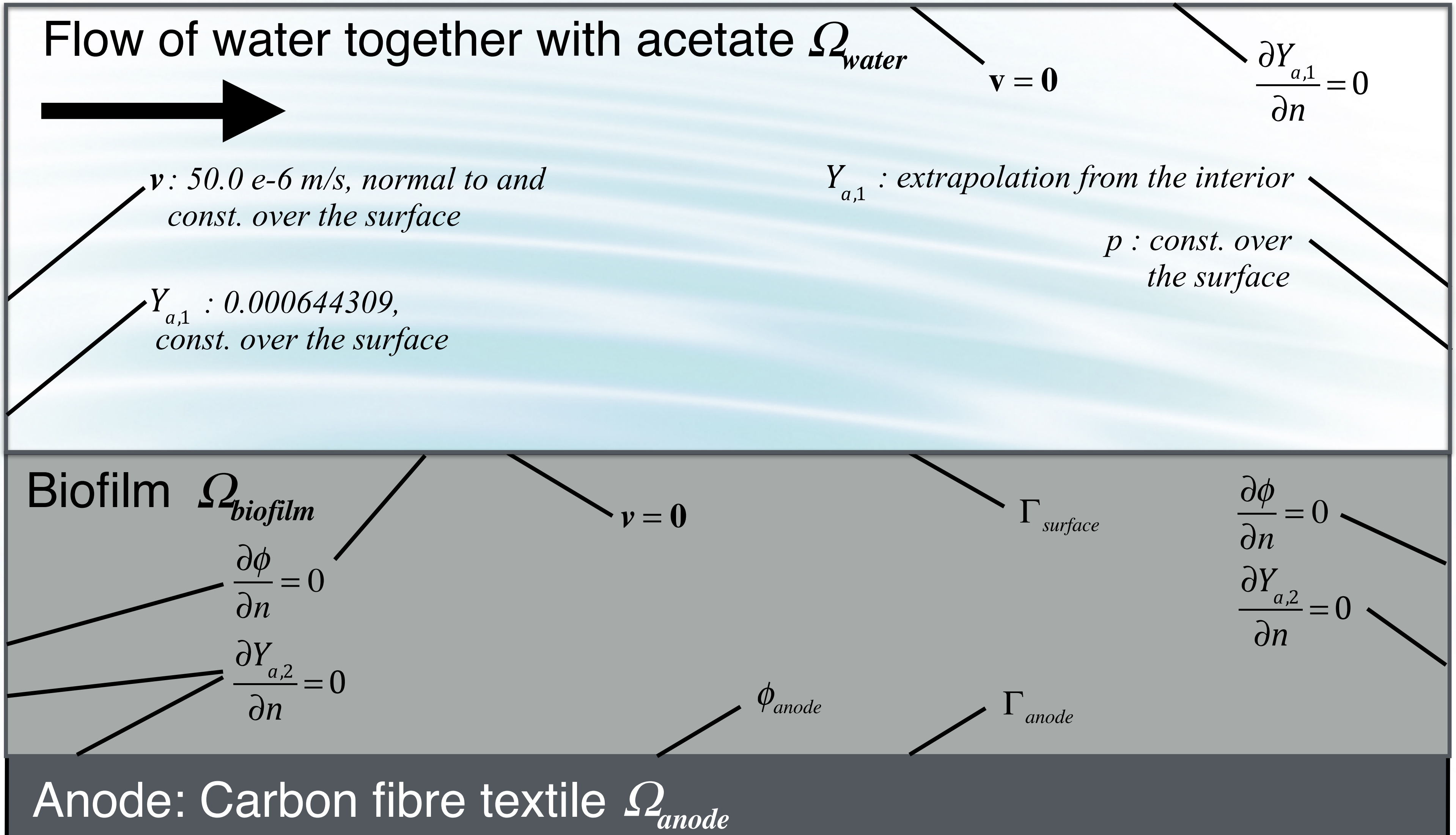


$$Y_{a,2}\big|_{wall} = Y_{a,1}\big|_{wall} = Y\big|_{wall}$$

$$Y\big|_{wall} = \frac{1}{\dfrac{\rho_2 D_{a,2}}{\rho_1 D_{a,1}}\dfrac{\Delta s_{water}}{\Delta s_{biofilm}}+1} Y_{a,1}\big|_{cell} + \frac{1}{\dfrac{\rho_1 D_{a,1}}{\rho_2 D_{a,2}}\dfrac{\Delta s_{biofilm}}{\Delta s_{water}}+1} Y_{a,2}\big|_{cell}$$

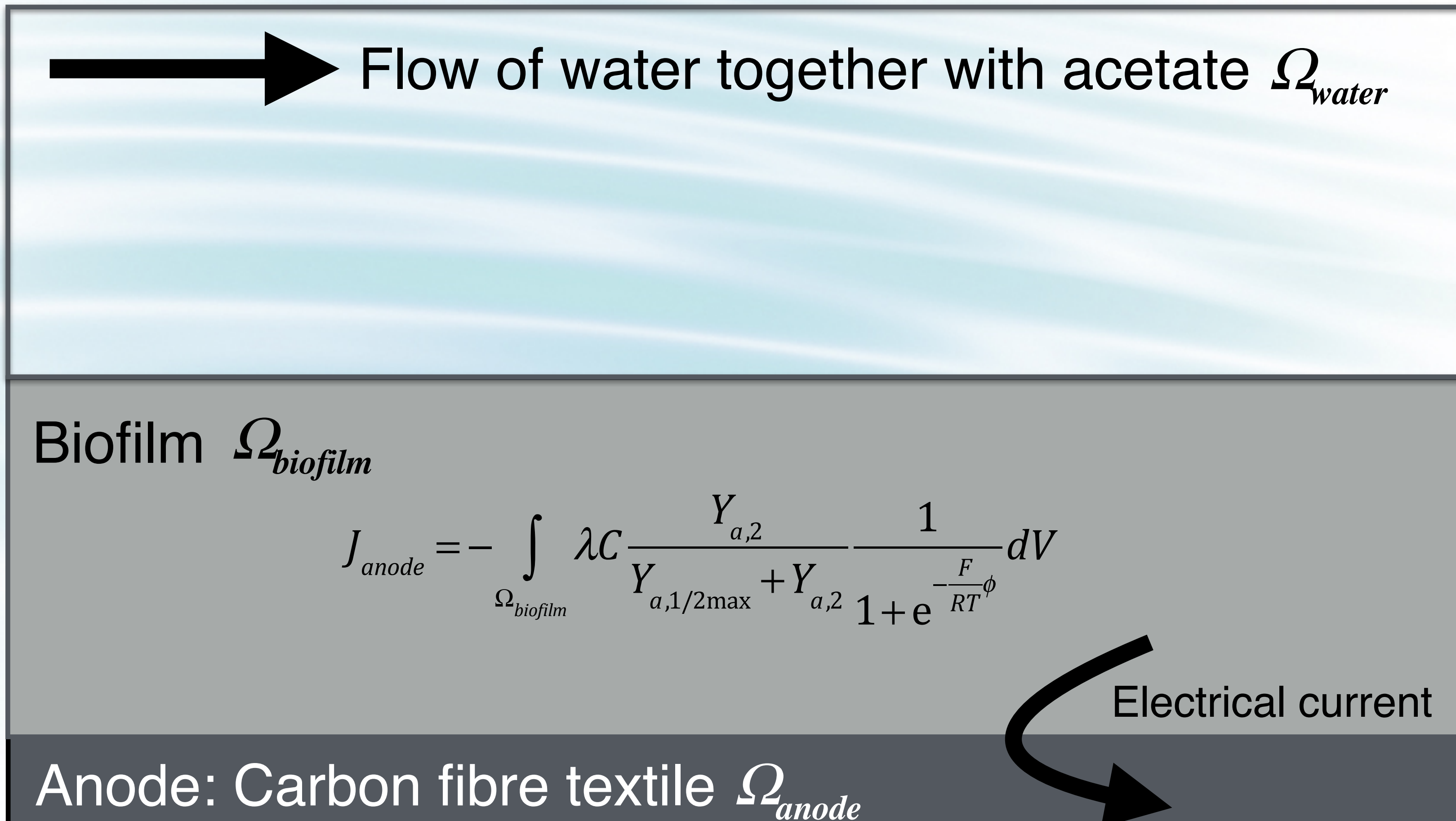
Mathematical Model - 5

- **Boundary conditions**



Mathematical Model - 6

- **All electrons produced in the biofilm must pass through the anode**



Mathematical Model - 7

- **Material properties at 37 °C**

Flow of water together with acetate Ω_{water}

Water: $\rho_{w,1} = 993.31 \frac{kg}{m^3}$ Acetate: $\rho_{a,1} = 993.31 \frac{kg}{m^3}$ VDI-Wärmeatlas (2002) Karat et al. (2008)

Water together with acetate: $\mu_1 = 692.78 \cdot 10^{-6} \frac{kg}{ms}$ VDI-Wärmeatlas (2002) Karat et al. (2008)

Diffusion coefficient: $D_{a,1} = 1.4697 \cdot 10^{-9} \frac{m^2}{s}$ Compton and Hancock (1999) Stewart (2003), Cussler (2009)

Biofilm $\Omega_{biofilm}$

Biofilm: $\rho_{b,2} = 1{,}010.00 \frac{kg}{m^3}$ Zhang and Bishop (1994)

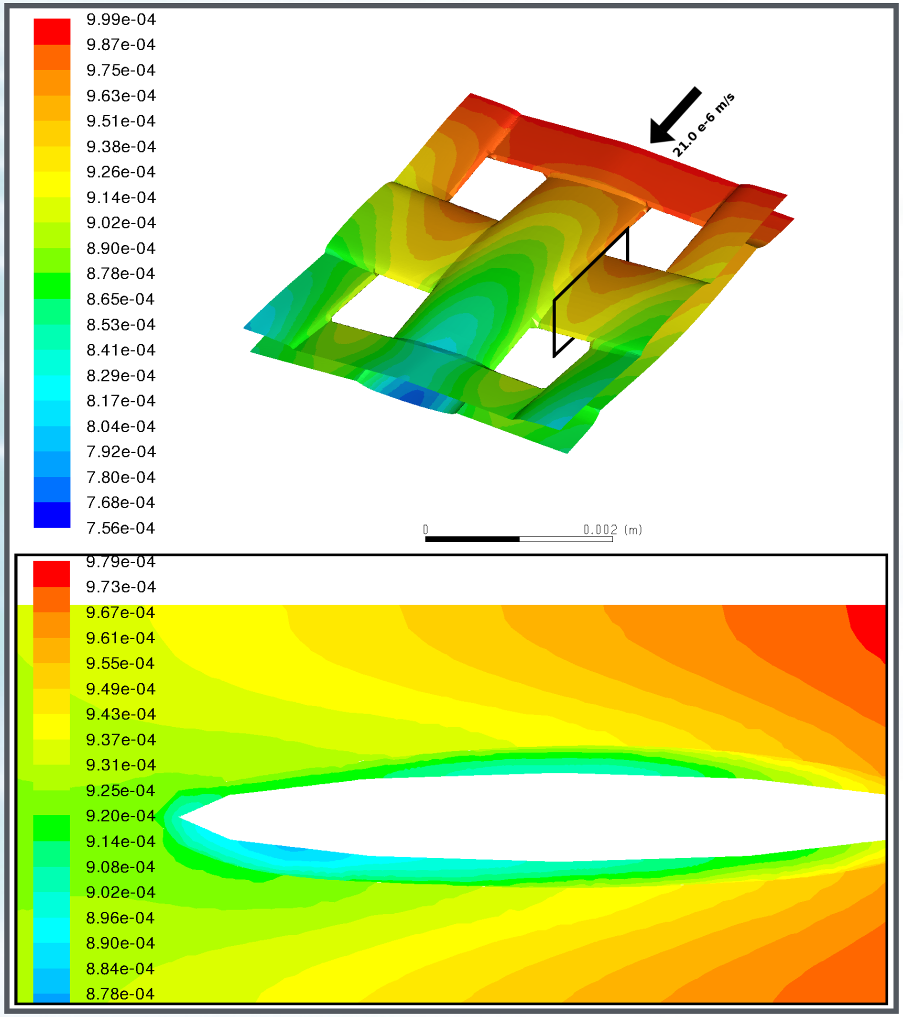
Acetate: $\rho_{a,2} = 993.31 \frac{kg}{m^3}$ Karat et al. (2008) VDI-Wärmeatlas (2002)

Diffusion coefficient: $D_{a,1} = 1.34110 \cdot 10^{-9} \frac{m^2}{s}$ Stewart (2003) Cussler (2009)

Anode: Carbon fibre textile Ω_{anode}

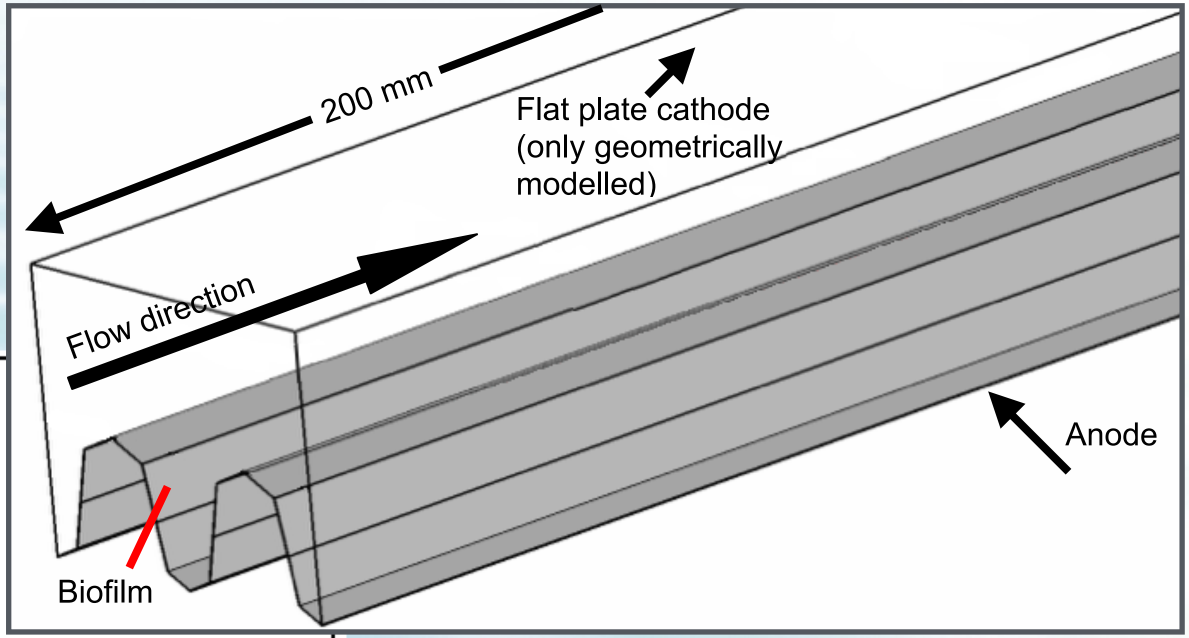
Mathematical Model - 8

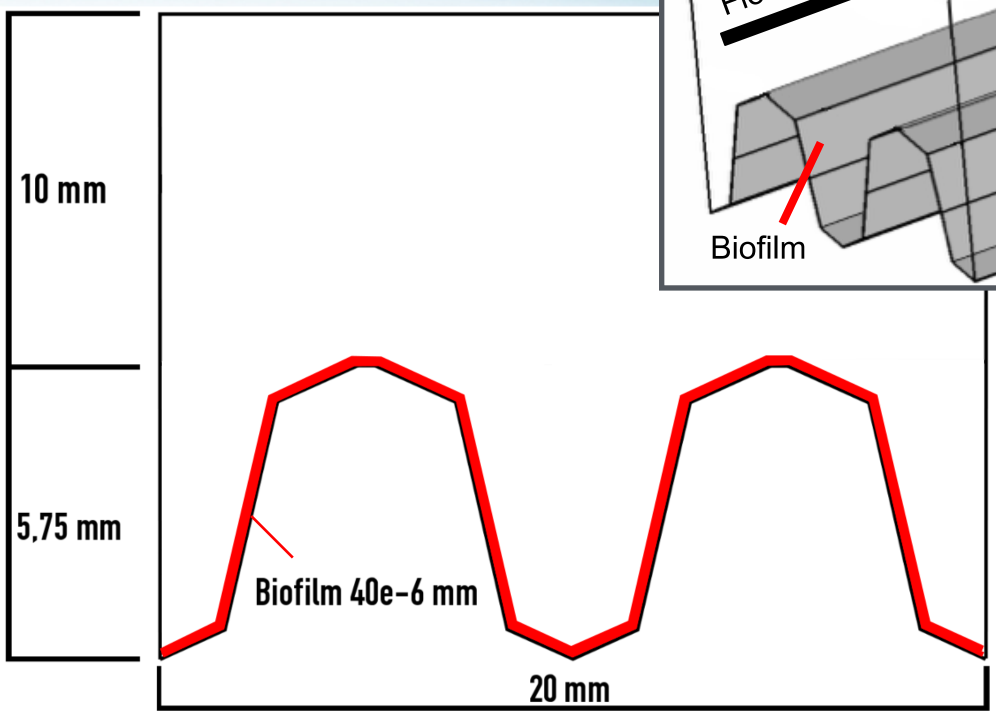
- This mathematical model was applied with validation to small geometrical structures of different carbon fibre textiles (Farber et al. 2019)
- Result: Surface of biofilm per volume of fabric dominates mass transfer
- Qualitatively validated by experiments
- Figure: Mass fraction of acetate on surface of biofilm



Mathematical Model - 9

- **Application of the mathematical model to half length of the full anode of 400 mm**





Inlet mass fraction acetate:	0,000644309
Inlet velocity:	0,00005 m/s
Temperature:	37 °C

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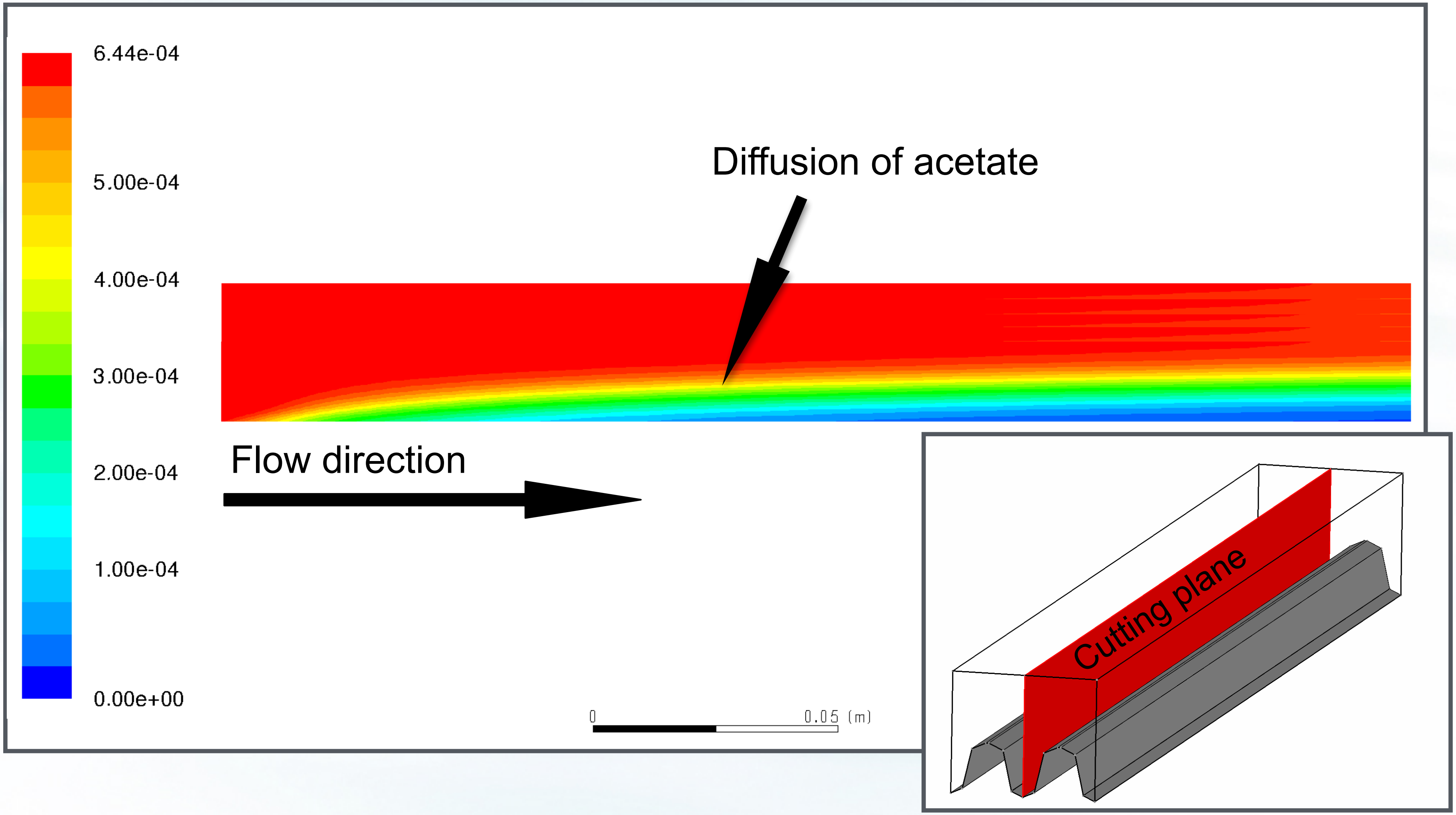
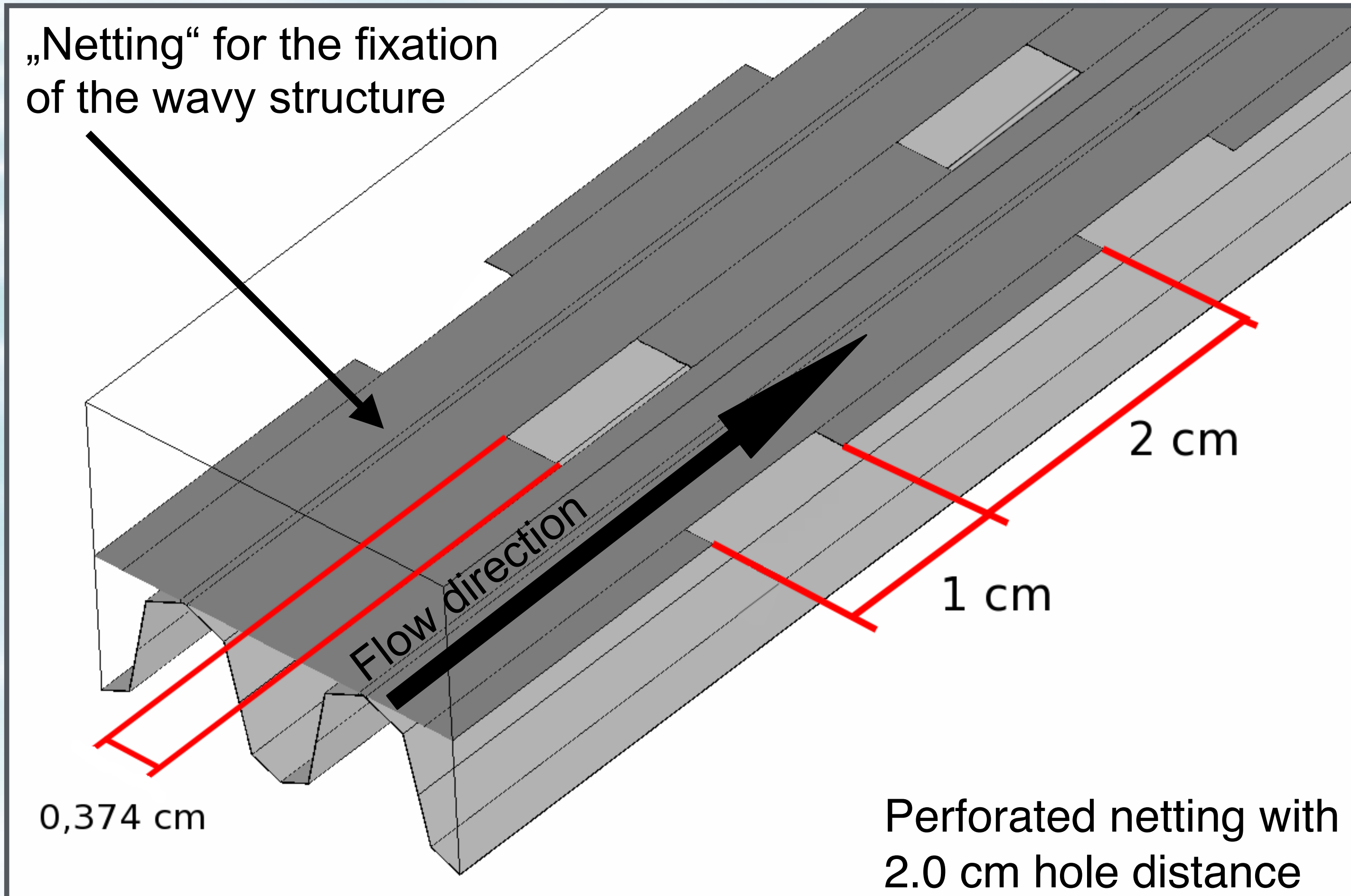
Results - 1

- **Mass fraction of acetate in cutting plane - diffusion is the dominating mass transfer mechanism**



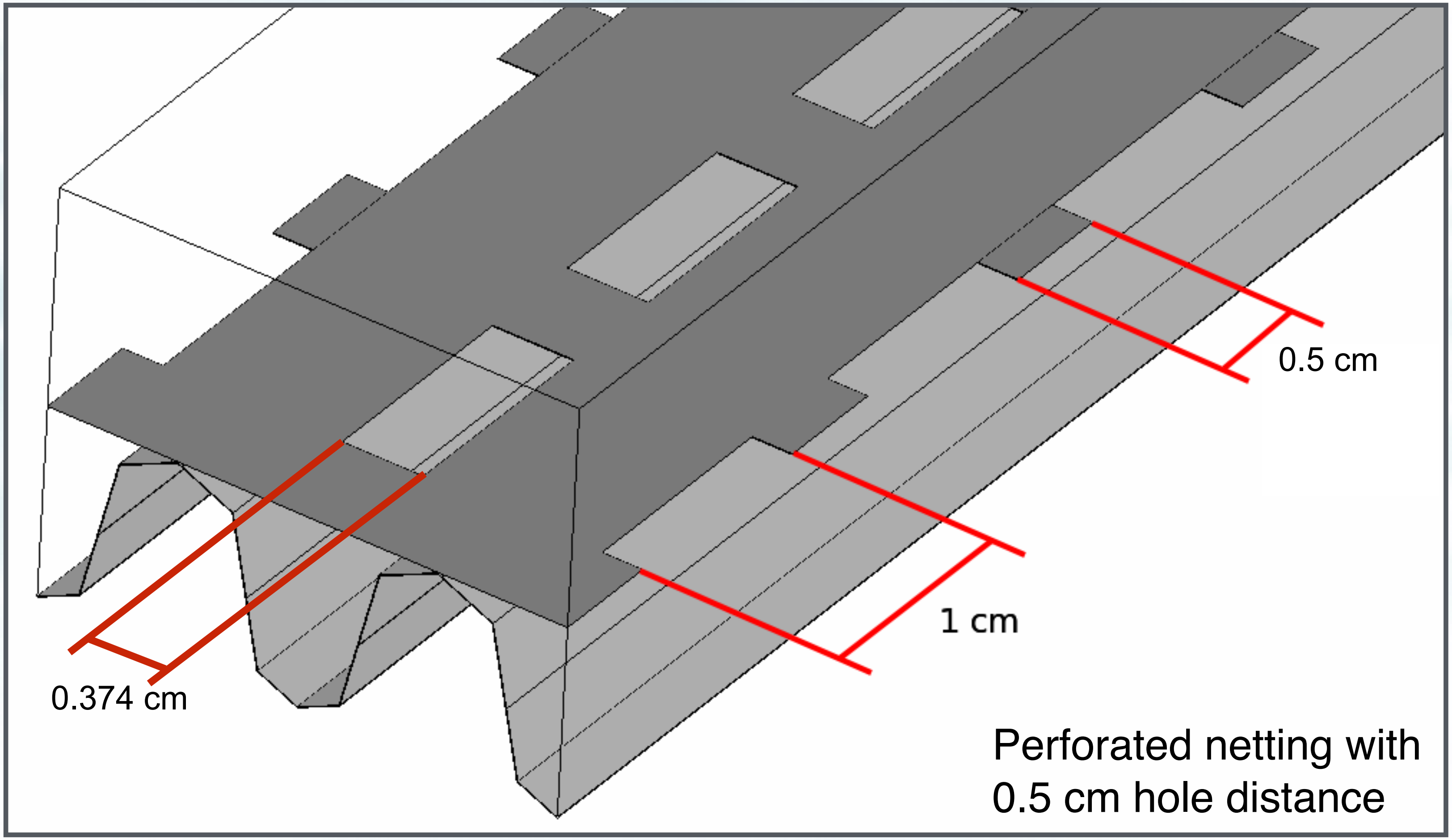
Results - 2

- **Production restrictions forced us to use an open structured textile web upon the anode to fix the wavy structure of the anode**



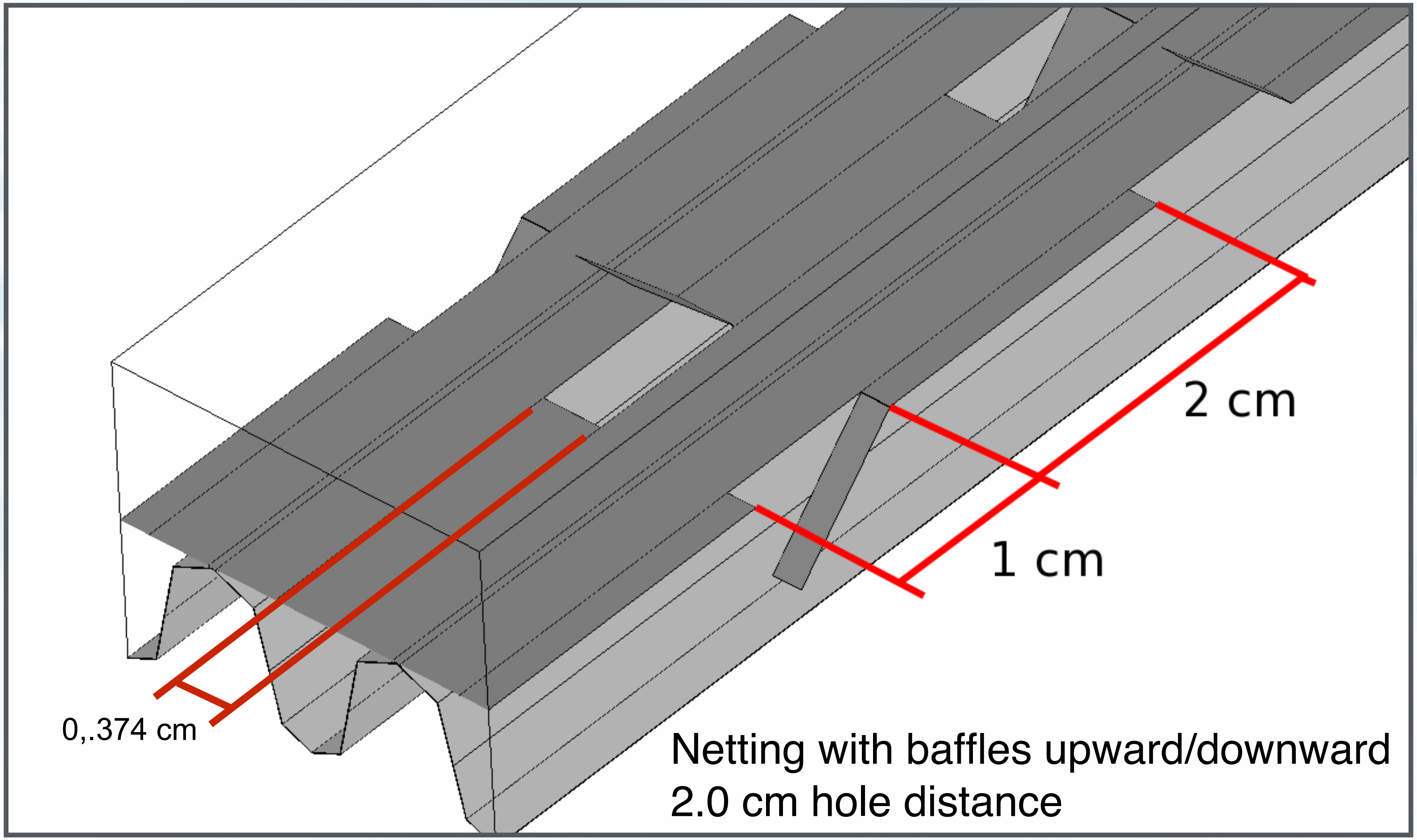
Results - 3

- In order to enhance cross flow diffusion the distance between holes was lowered



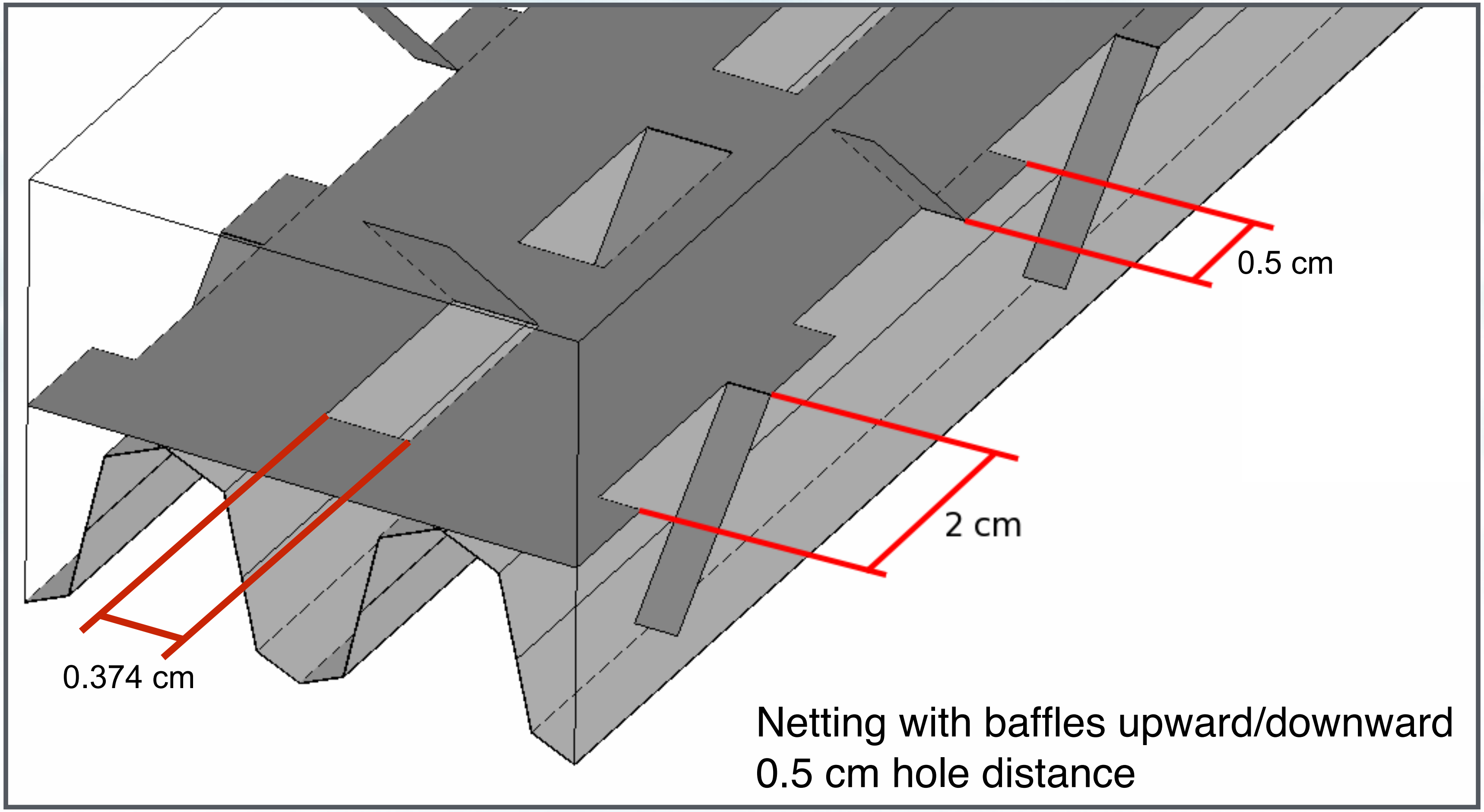
Results - 4

- **In order to enhance cross flow further upward/ downward baffles were introduced**



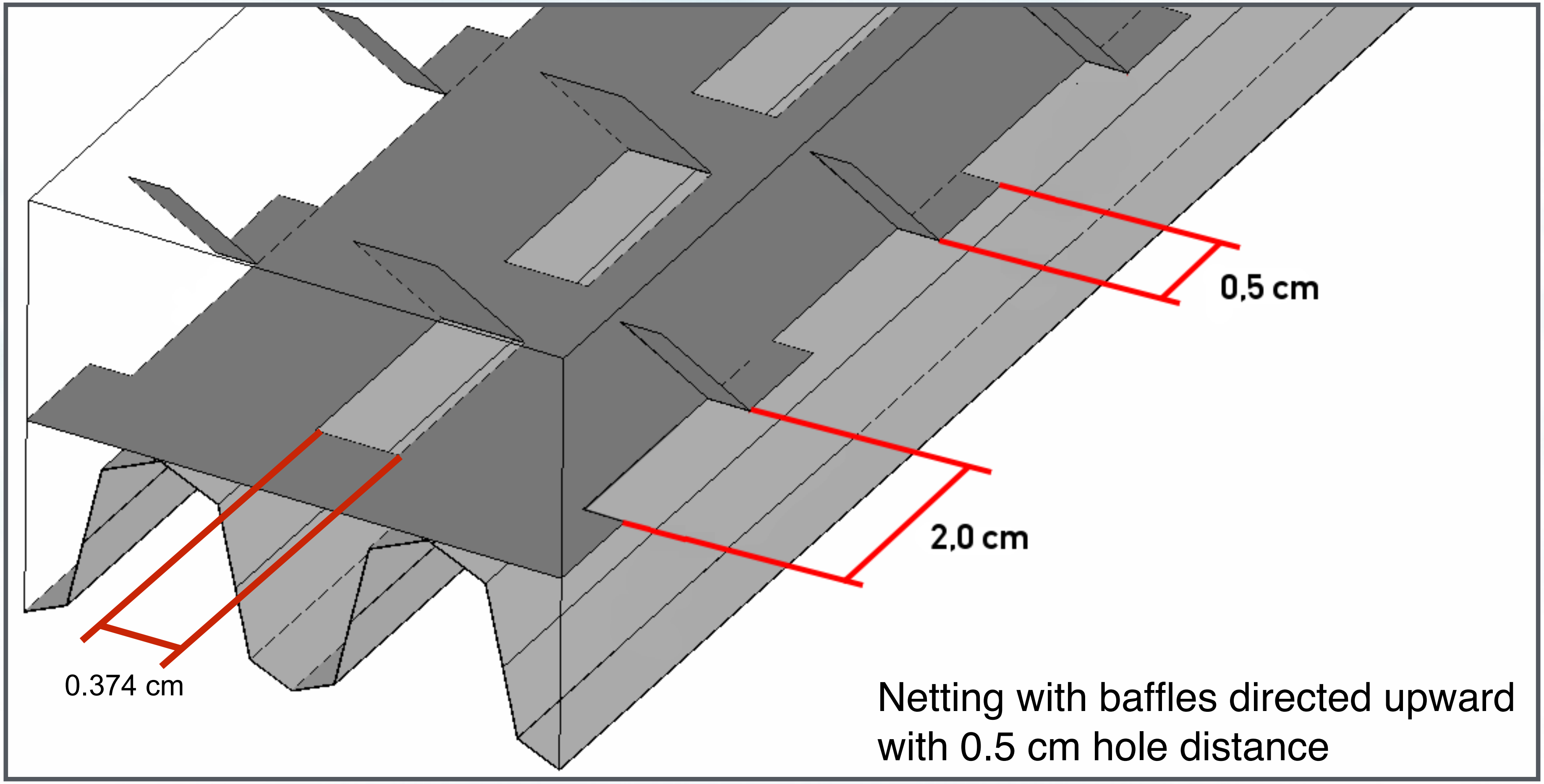
Results - 5

- **For better cross flow the distance between holes was reduced**



Results - 6

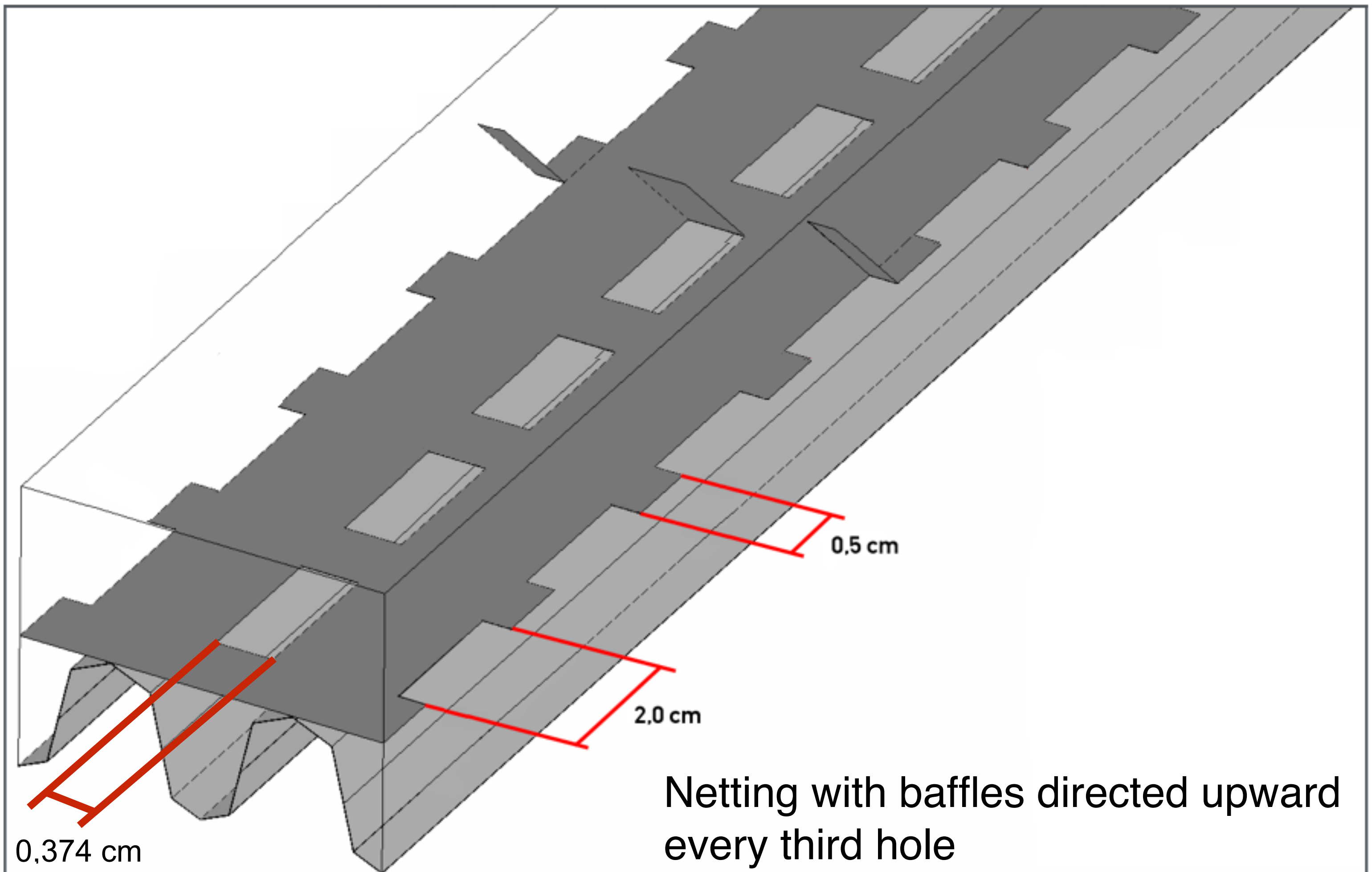
- **Further geometrical modifications**



Netting with baffles directed upward with 0.5 cm hole distance

Results - 7

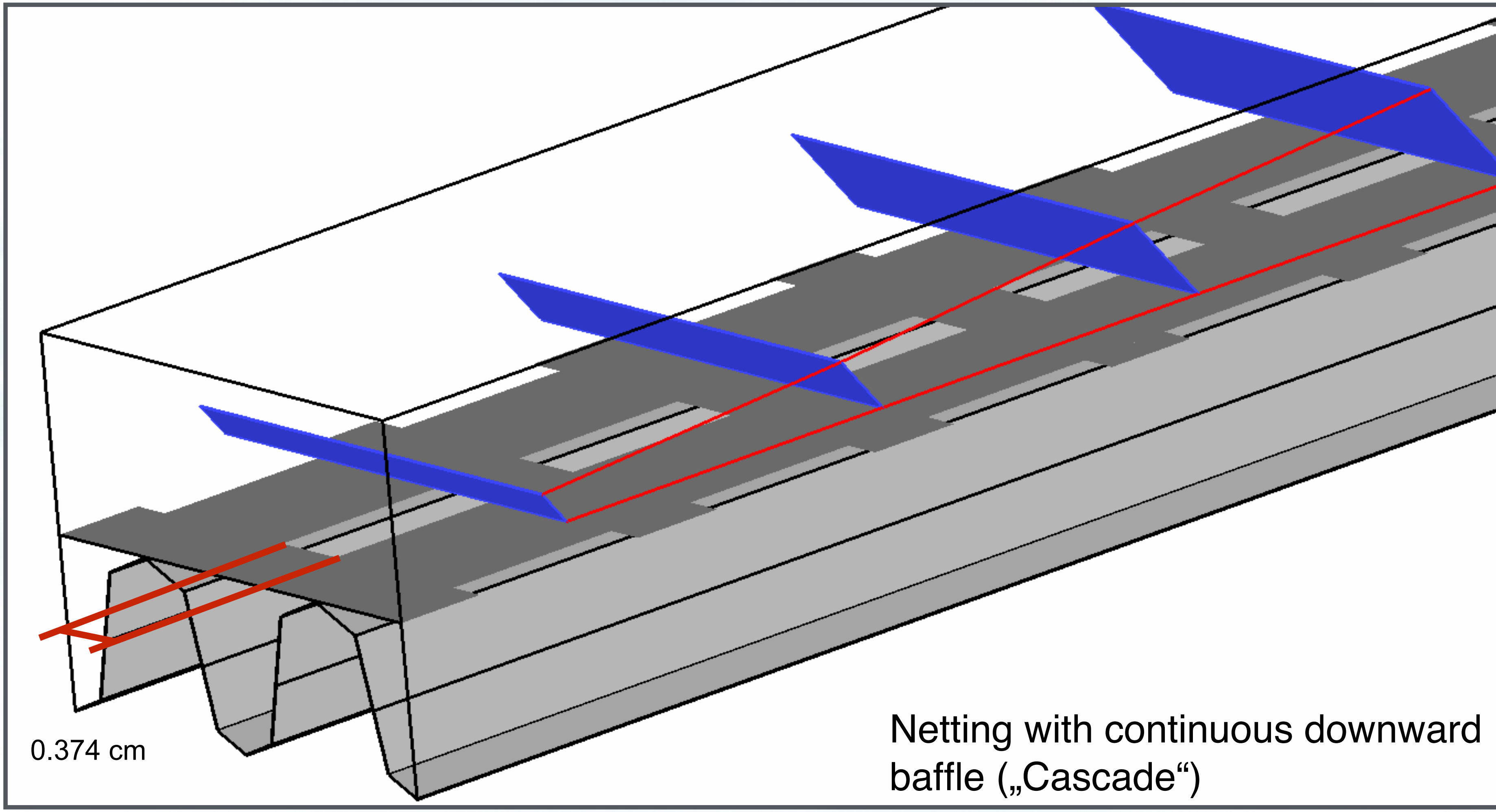
- **Geometrical modifications cont'd**



Netting with baffles directed upward every third hole

Results - 8

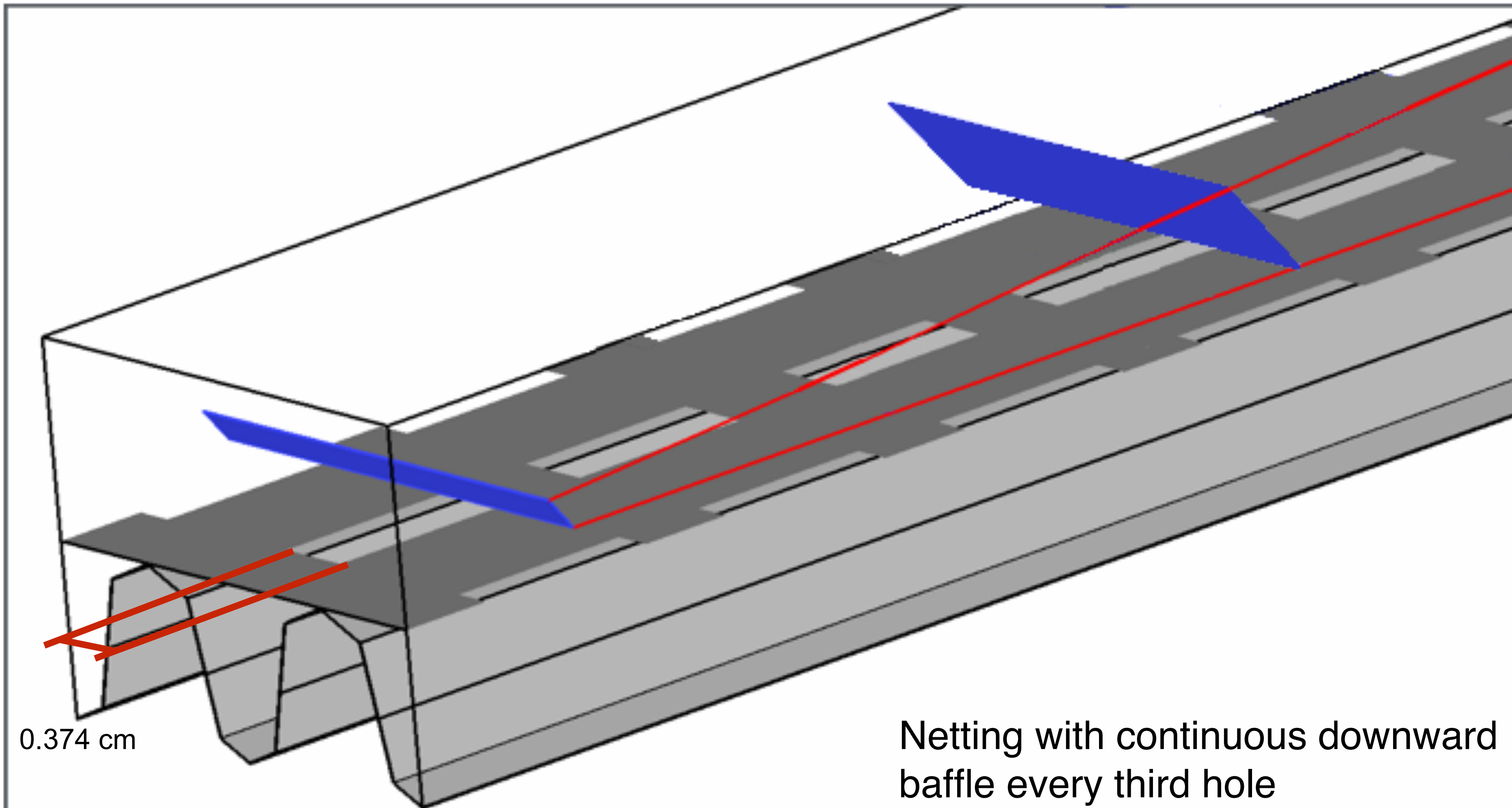
- **Geometrical modifications cont'd**



Netting with continuous downward baffle („Cascade")

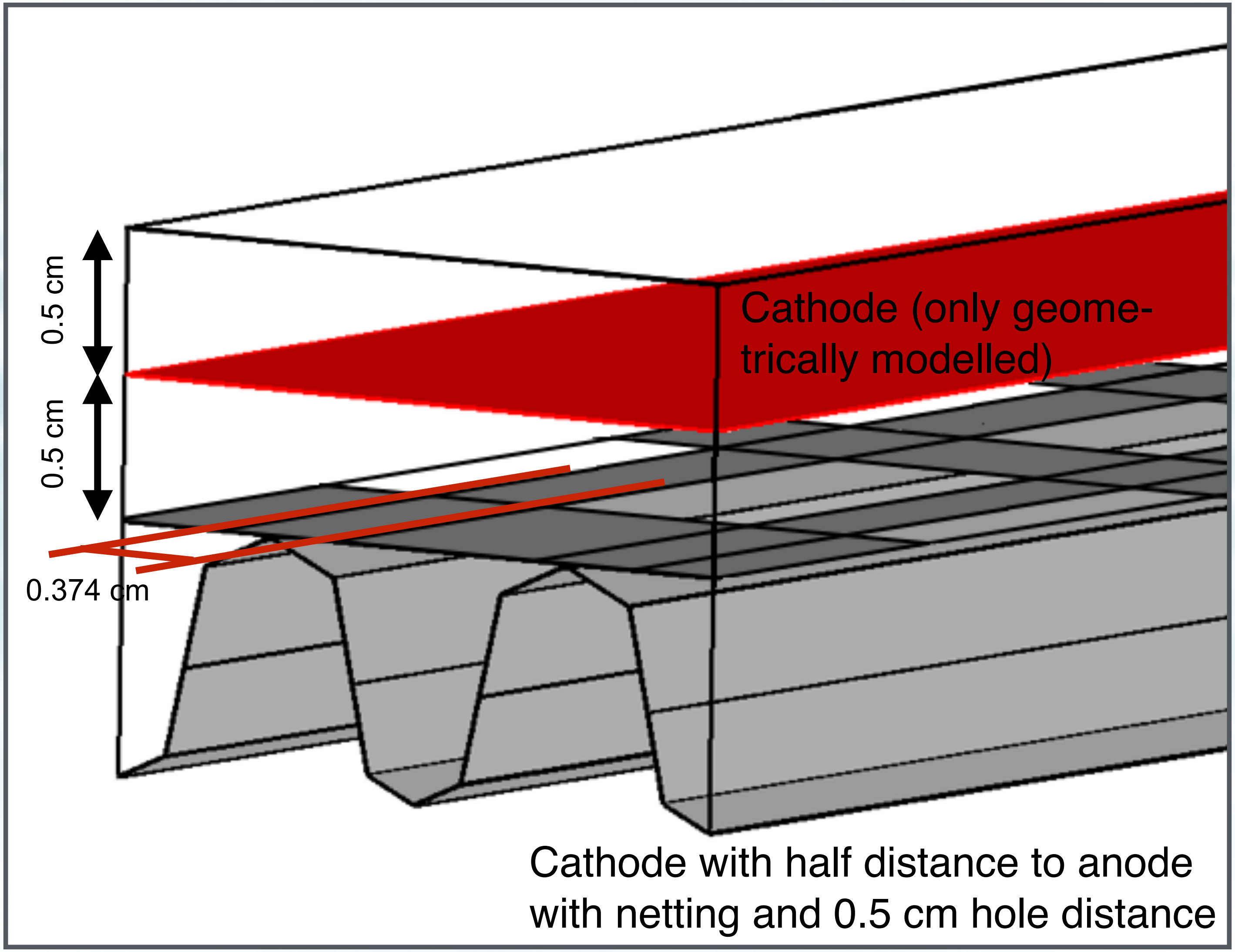
Results - 9

- **Geometrical modifications cont'd**



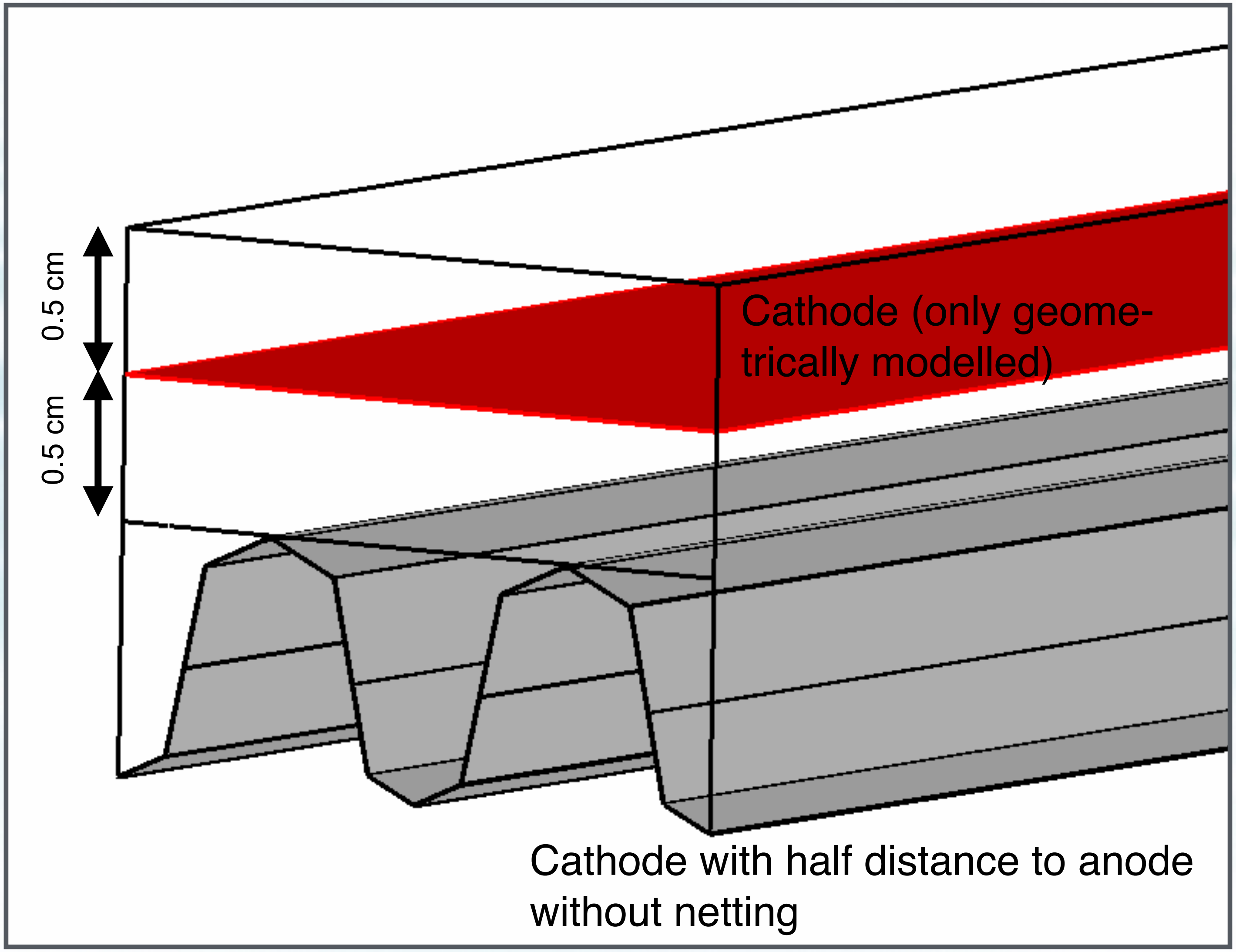
Results - 10

- **Geometrical modifications cont'd**



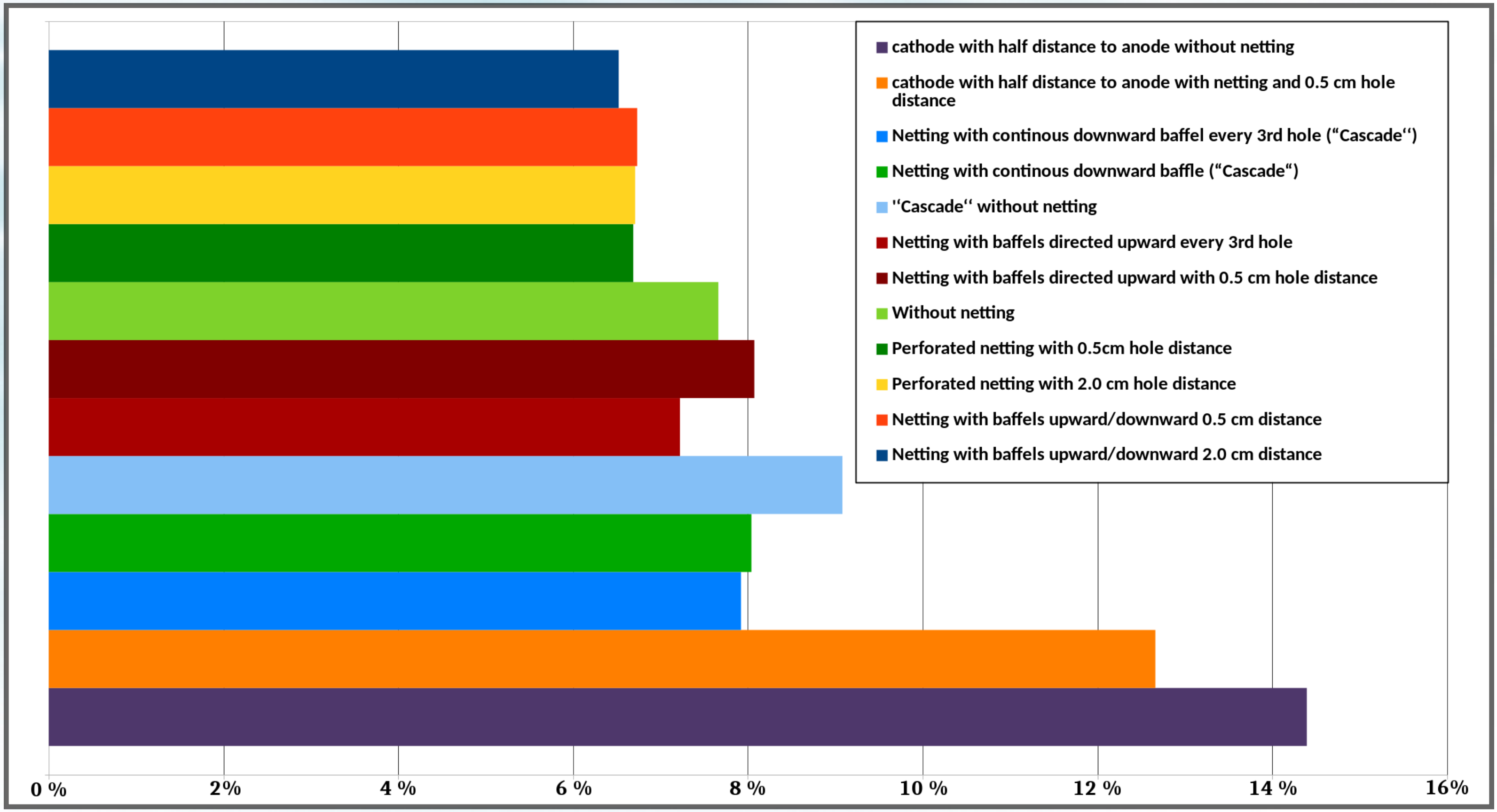
Results - 11

- **Geometrical modifications cont'd**



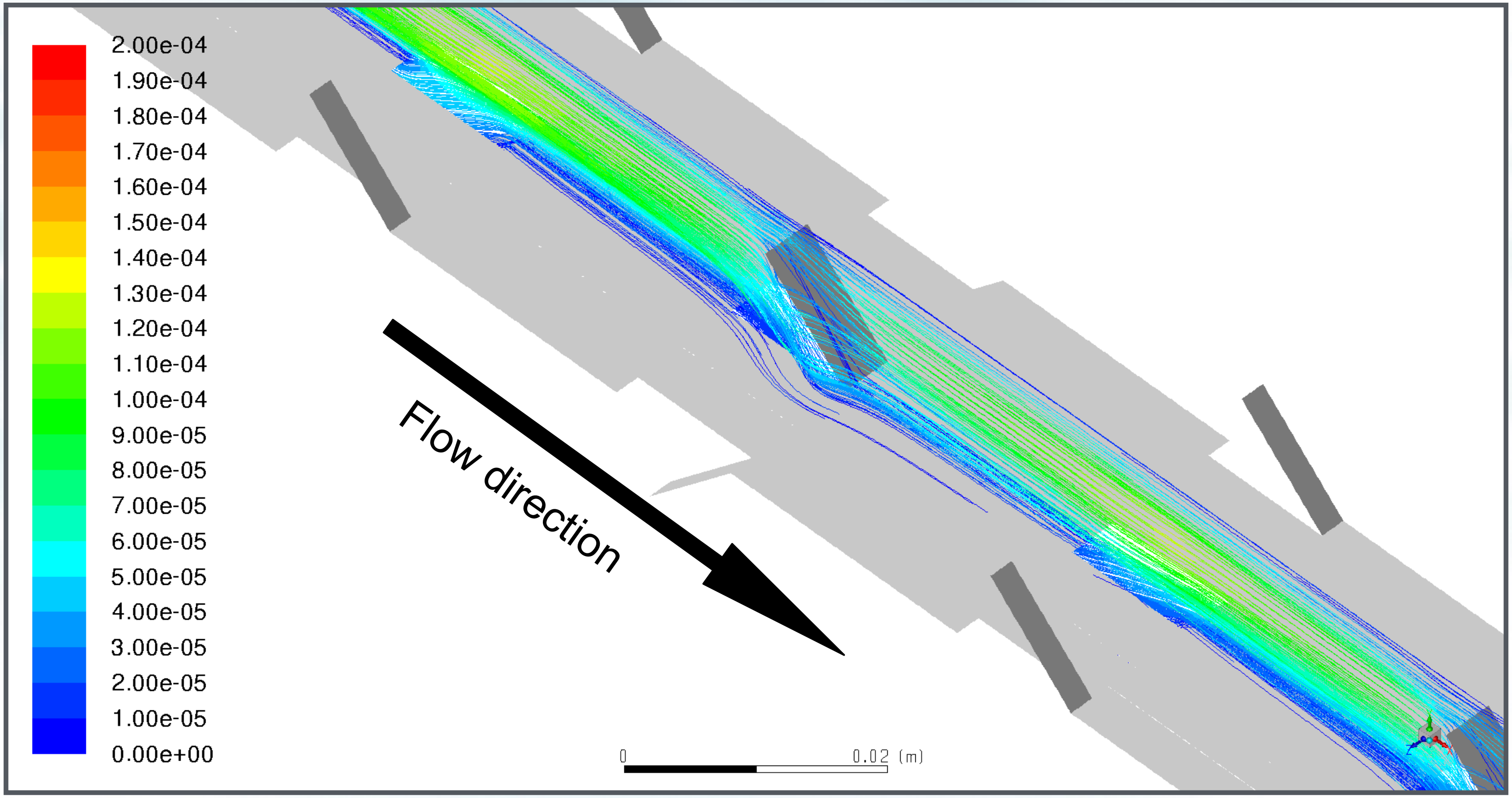
Results - 12

- Mass flux difference of acetate outlet to inlet in %
- Superiority of small distance is qualitatively validated by Cheng et al. (2006) and Ghangrekar and Shinde (2006)



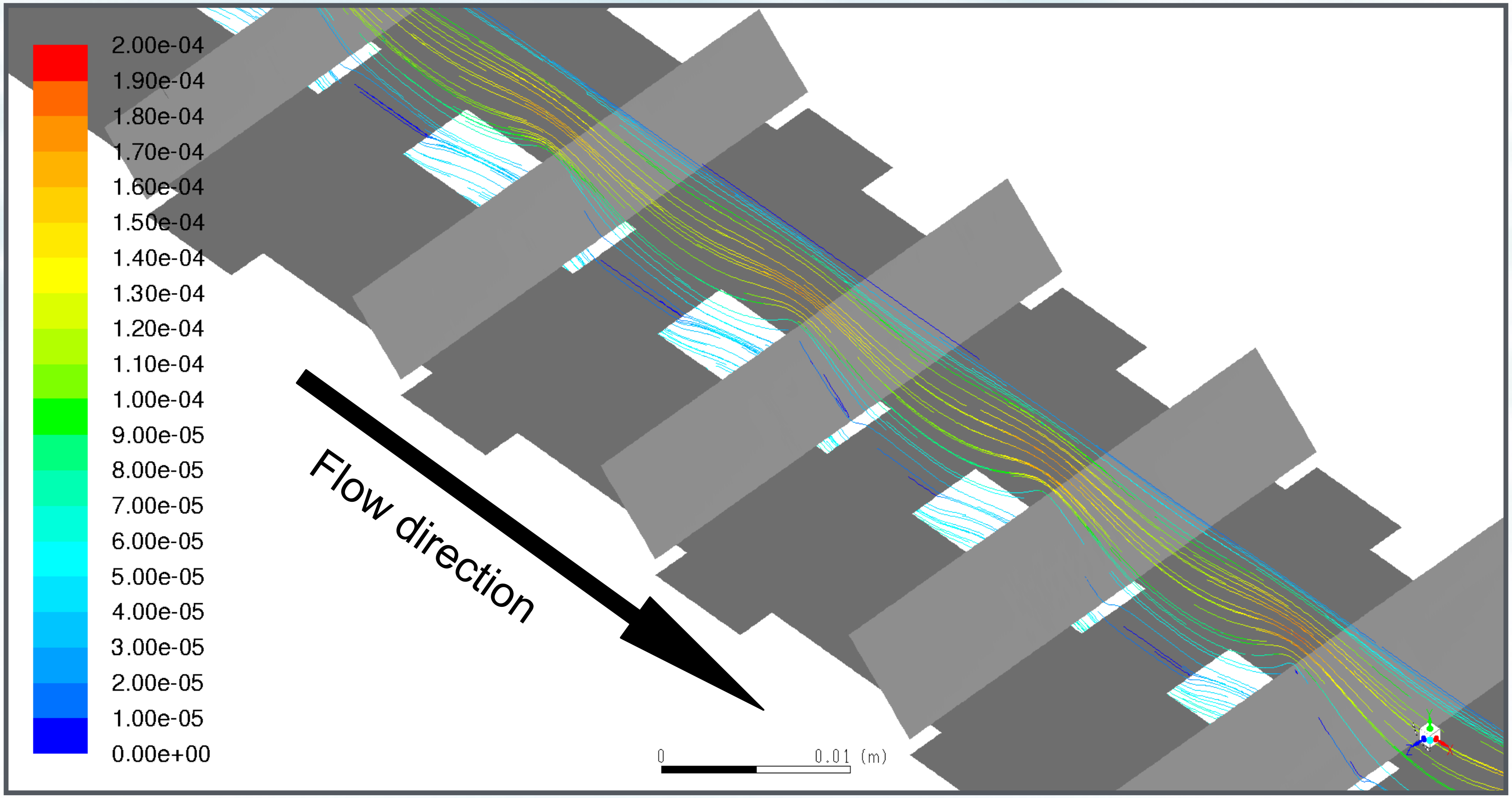
Results - 13

- **Pathlines of flow coloured with velocity magnitude**
- **Water with acetate flows around the baffle and is only marginally guided to the anode**



Results - 14

- **Pathlines of flow coloured with velocity magnitude**
- **The cascade is not successful enough to guide fresh fluid to the anode**



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Conclusion

- A mathematical model mass transfer of acetate to the anode of a MFC was developed
- The model allows an in-depth analysis of mass transfer to the anode of the MFC
- Mass transfer is dominated by cross-flow diffusion
- Several geometrical configurations were tested to bring „fresh fluid“ to the surface of the anode
- The configurations didn’t show any significant difference, except halving the distance anode-cathode
- This could increase electricity generation per volume of the MFC significantly

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