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Seeking minimum entropy production for flow-field patterns and geometries in fuel cells

Marco Sauermoser, Signe Kjelstrup, Natalya Kizilova, Eirik Grude Flekkøy, Bruno G. Pollet

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Summary

- Aim:
  - Optimize tree-shaped flow field pattern for PEMFCs by minimizing the entropy production (EP).
  - Find design criteria

- Method:
  - 1D calculations using analytic pressure drop and EP in MATLAB
  - 3D simulations with OpenFoam’s simpleFoam solver

- Results:
  - Larger width scaling parameters than the one from Murray’s Law give lower entropy production
  - Channel width has the biggest influence on entropy production
  - Peclet number analysis gives range of current densities to use

PEM fuel cell

- PEM= Proton exchange membrane or polymer electrolyte membrane
- Core element: ion exchange membrane (mostly Nafion)
- Fuel: H_2 & O_2
- Exhaust: H_2O + excess gases

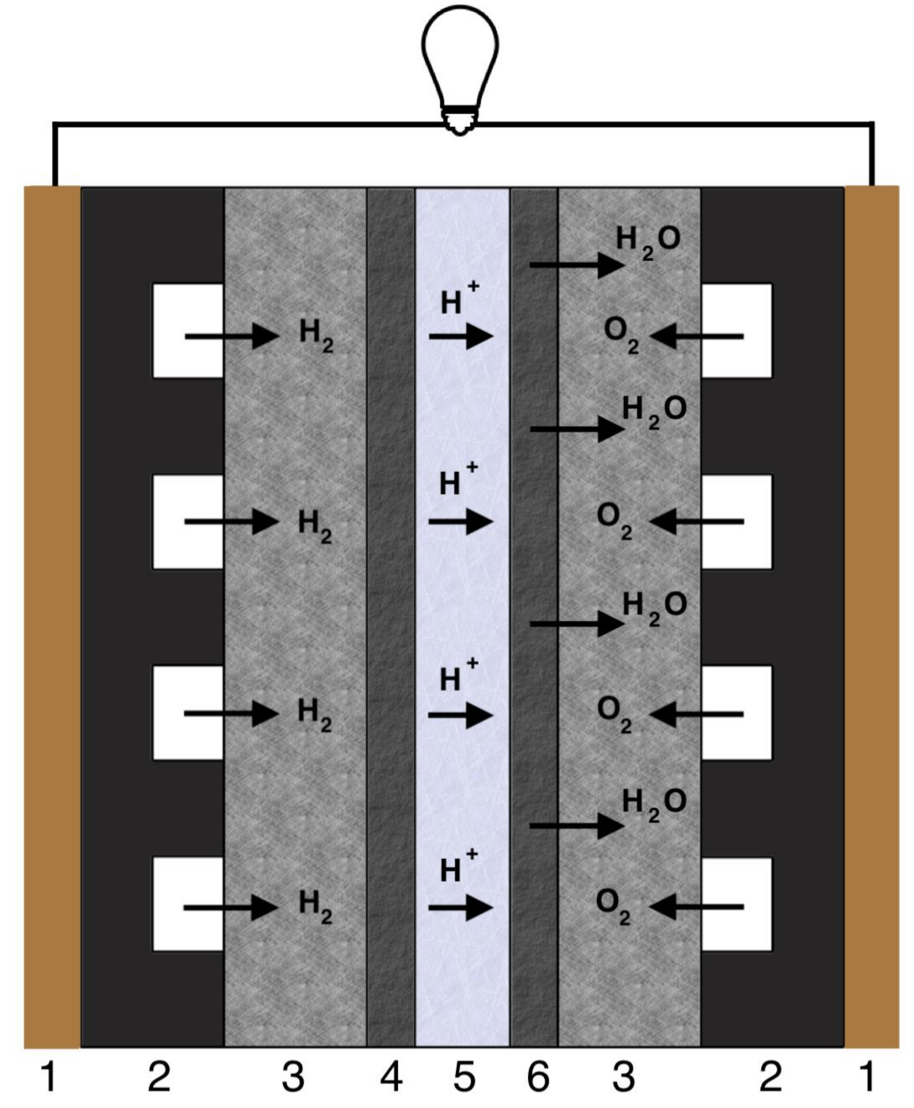
Anode: $H_2(g) \rightarrow 2H^+(aq) + 2e^-$

Cathode: $\frac{1}{2}O_2(g) + 2H^+(aq) + 2e^- \rightarrow H_2O(l)$

Overall: $H_2(g) + \frac{1}{2}\, O_2(g) + t_w\, H_2O\,(l) \rightarrow (t_w+1)\, H_2O(l)$

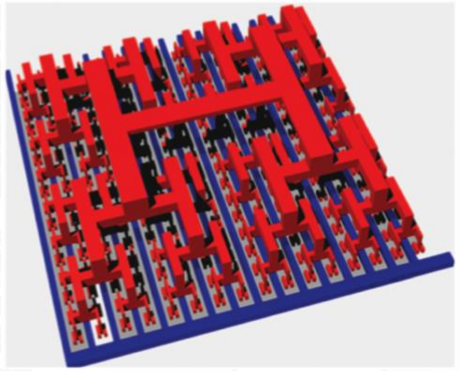
PEM fuel cell

- 1 – Current collector
- 2 – Flow field plate
- 3 – Gas diffusion layer (GDL)
- 4 – Anode
- 5 – Membrane
- 6 – Cathode

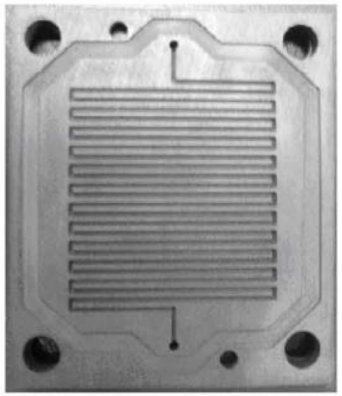


Introduction

- Tree-shaped patterns proven to increase performance of PEMFCs compared to serpentine patterns [1]
- Uniform outlet flow rate to achieve uniform fuel distribution
- Murray’s Law for scaling should deliver minimum EP [2]
- One of the goal is to have Pe<1 at the outlet



Tree-shaped FFP [1]



Serpentine FFP [3]

[1] P. Trogadas, J. I. S. Cho, T. P. Neville, J. Marquis, B. Wu, D. J. L. Brett, and M.-O. Coppens. A lung-inspired approach to scalable and robust fuel cell design. Energy Environ. Sci., 11(1), 2017.
[2] S. Gheorghiu, S. Kjelstrup, P. Pfeifer and M.-O. Coppens. Is the lung an optimal gas exchanger? In: Fractals in Biology and Medicine, ed. G. A. Losa, D. Merlini, T. F. Nonnenmacher and E. R. Weibel, Birkhauser Basel, Basel, 2005, pp. 31–42.
[3] Hong Liu, Peiwen Li, Daniel Juarez-Robles, Kai Wang, and Abel Hernandez-Guerrero. Experimental Study and Compari- son of Various Designs of Gas Flow Fields to PEM Fuel Cells and Cell Stack Performance. Frontiers in Energy Research, 2014.

Questions

- Questions:
  - Is Murray's law the most efficient scaling for FCs?
  - How does the width influence the entropy production?
  - How can you estimate the exact pressure drop in the most accurate way?
  - Can we define a design criterion based on the Peclet number?

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1D tree-shaped flow field pattern

$$l_{j,i} = \frac{1}{2^{j/k}} l_0$$

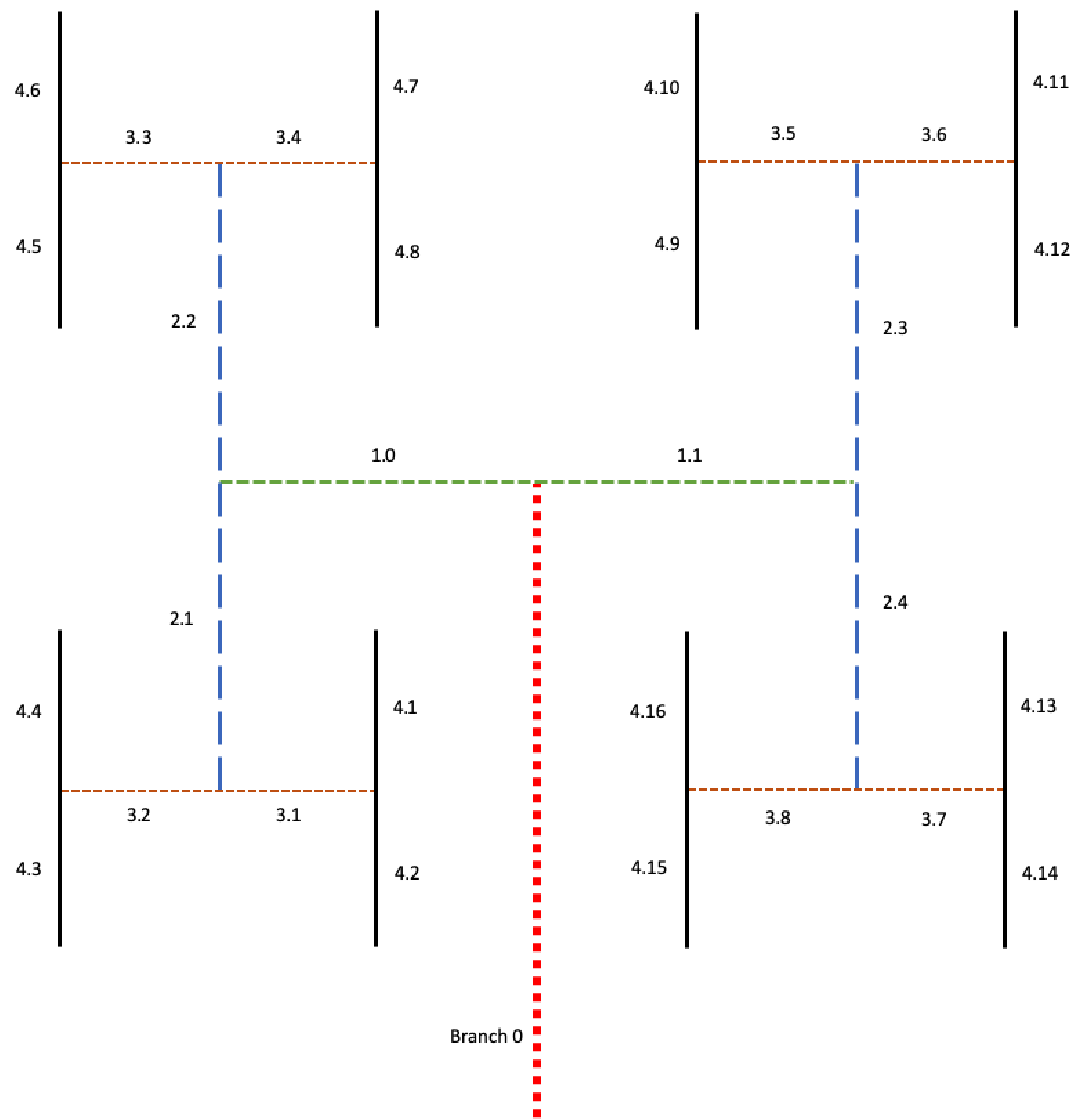
$$w_{j,i} = a^j w_0$$

$$Q_{j,i} = \frac{1}{2^j} Q_0$$

$$\left(\frac{dS_{irr}}{dt}\right)_{j,i} = -Q_{j,i} \frac{\Delta p_{j,i}}{T}$$

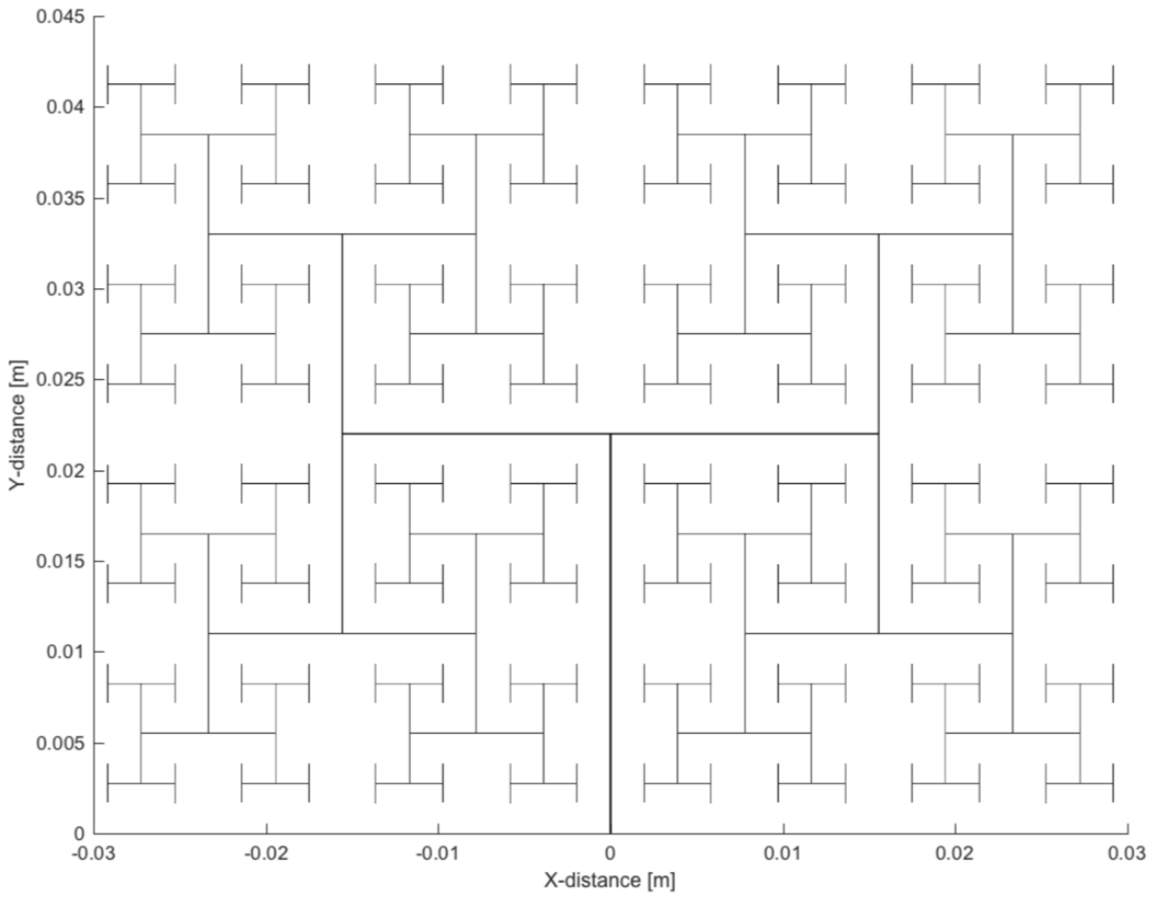
$$\frac{dS_{irr,spec.}}{dt} = \frac{dS_{irr}}{dt} w_{j,i}^{-1}$$

- Rectangular channels
- constant depth

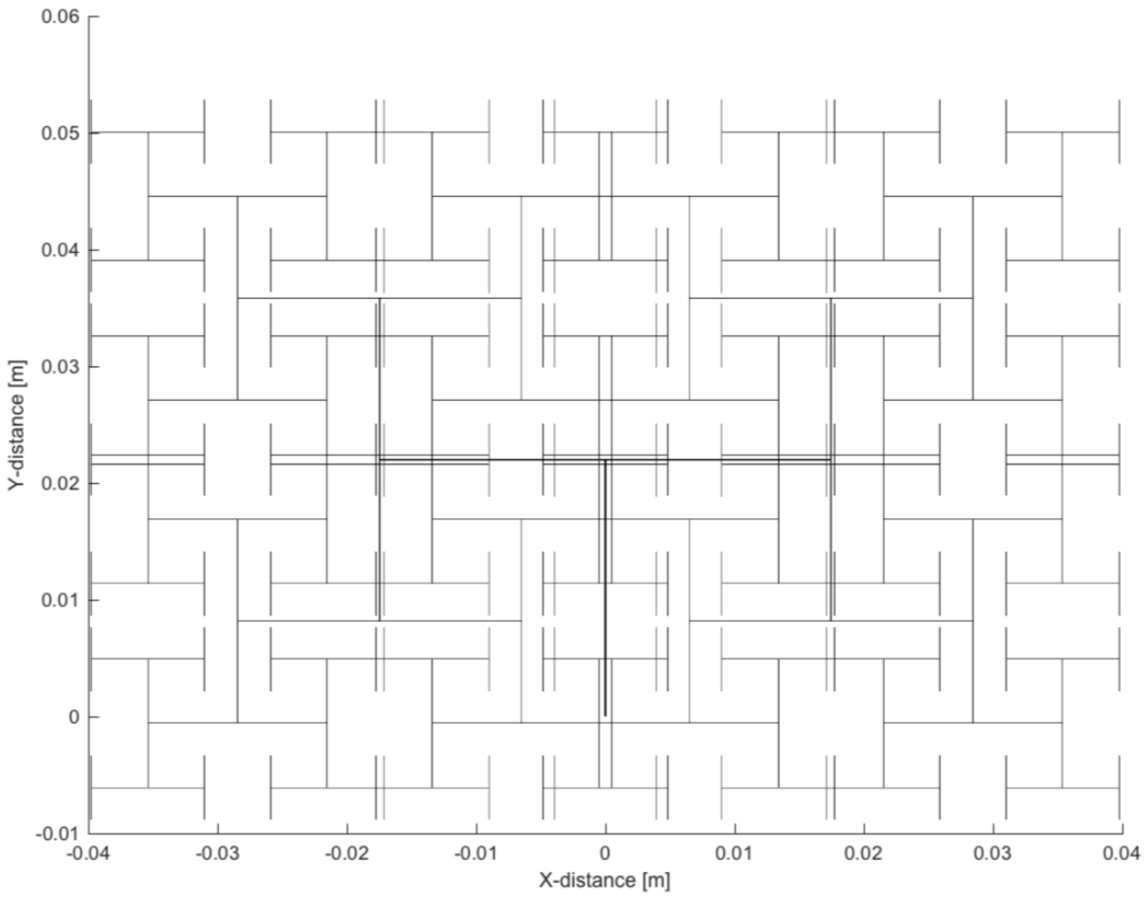


1D tree-shaped flow field pattern

k=2

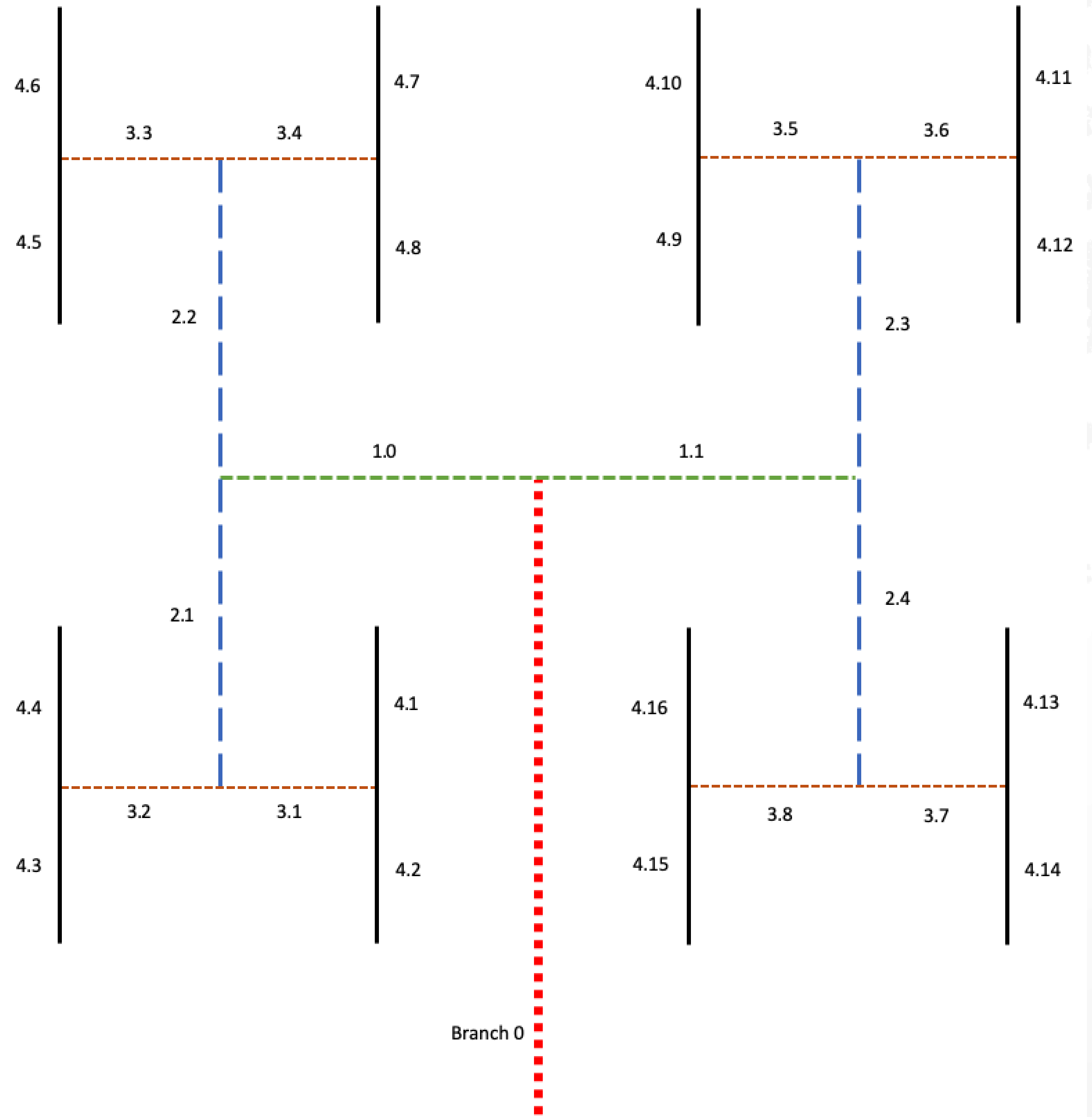


k=3



1D tree-shaped flow field pattern

- If lengths are scaled:
  - Rectangular area
  - Can have crossovers
- Therefore→no length scaling
- Space filling (25cm^2):
  - Gen. 0: *l*=24mm
  - Gen. 1: *l*=12mm
  - Gen. 2: *l*=12mm
  - Gen. 3: *l*=6mm
  - Gen. 4: *l*=6mm



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1D – Pressure drop

$$\Delta p_{i,j} = -\frac{128\mu l_{i,j}}{\pi d_{i,j}^4} Q_{i,j}$$

- 3 different cases investigated
  - Hydraulic diameter ($d_{j,i}=D_{j,i}$)

$$D_{j,i} = \frac{2w_{j,i}h_{j,i}}{w_{j,i}+h_{j,i}}$$

  - Equivalent area

$$d_{j,i} = \sqrt{\frac{4}{\pi} w_{j,i} h_{j,i}}$$

  - Analytic solution of HP-flow for rectangular channels

$$\Delta p_{j,i} = -Q_{j,i}\frac{12\mu l_{j,i}}{h_{j,i}^3 w_{j,i}}\left[1-\sum_{n=0}^{\infty}\frac{192}{(2n+1)^5\pi^5}\frac{h_{j,i}}{w_{j,i}} tanh\left(\frac{2n+1}{2}\frac{\pi w_{j,i}}{h_{j,i}}\right)\right]^{-1}$$ [4]

[4] White, F. M. (2011). *Fluid Mechanics*. McGraw-Hill, 7 edition.

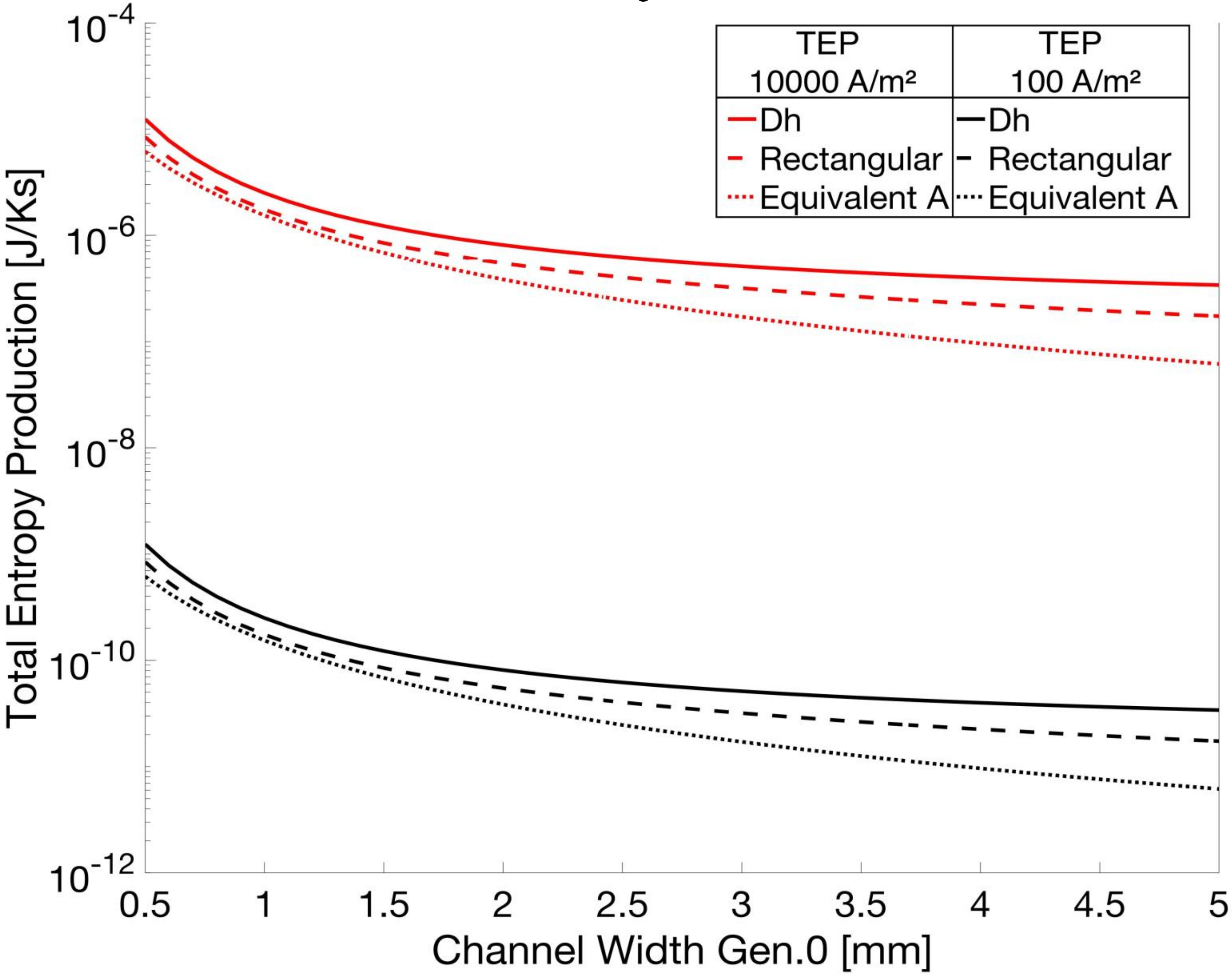
Case studies

Study	Investigation	Variables	Method
1	Flow rate & Δp calc. method dependency on TEP & TSEP	Flow rate, Δp calculation method, w_0	1D
2	Murray's Law and entropy production	a, w_0	1D
3	1D Δp	a, Δp calculation method	1D
4	Flow rate distribution	a, w_0	3D
5	3D TEP & TSEP	a, w_0, flow rate	3D
6	Comparison 1D & 3D Δp	a, Δp calculation method, 3D pressure drop	3D, 1D
7	Peclet number	characteristic length, w_0, a, flow rate	1D

1D – Total entropy production results

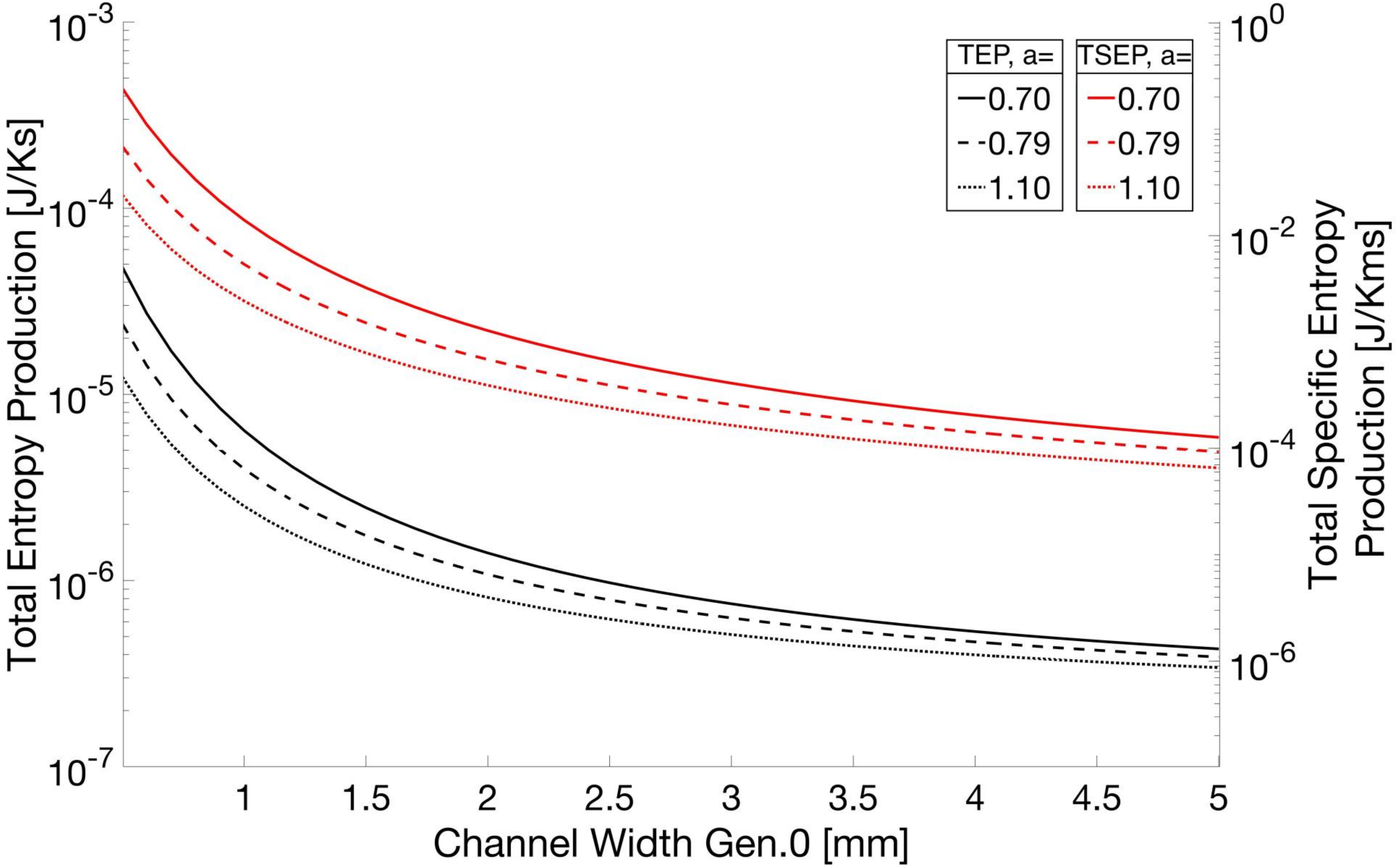
Current density $[A/m^2]$	Flow rate $[m^3/s]$
10000	5.7104×10^{-6}
5000	2.8552×10^{-6}
1000	5.7104×10^{-7}
100	5.7104×10^{-8}
10	5.7104×10^{-9}

w_0=1mm

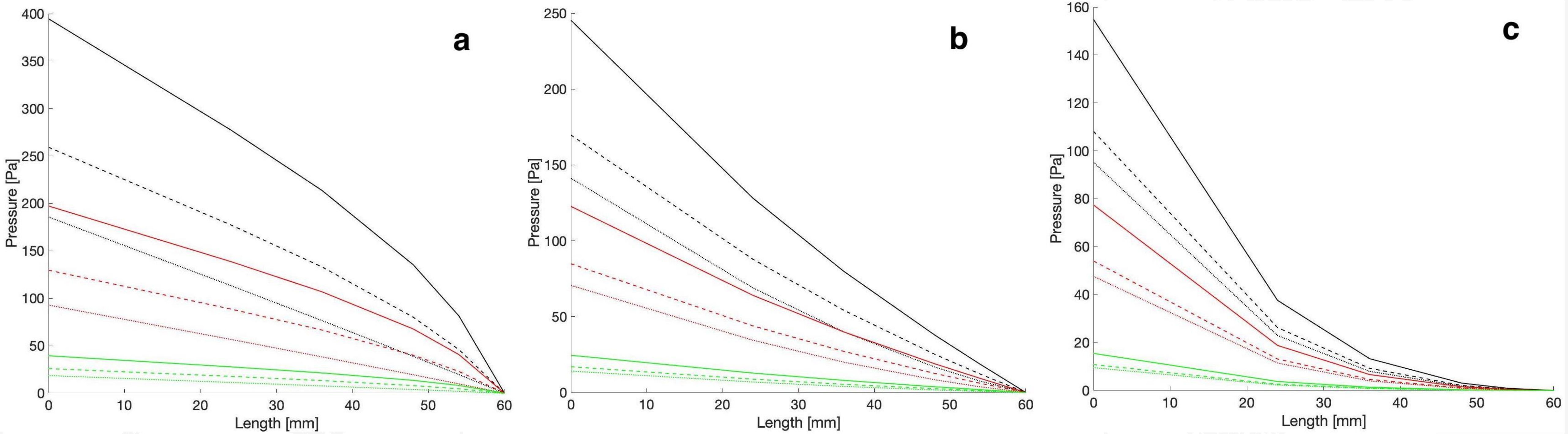


1D – Entropy production

w_0=1mm



1D – Pressure drop results



a. w_0=1mm a=0.70

b. w_0=1mm a=0.79

c. w_0=1mm a=0.90

1D – Summary

- Flow rate shifts entropy production to higher or lower values
- Murray's law does not give lowest entropy production values
- Strong dependency on width from 0.5 to 2mm
- Form of pressure curve changes with *a*
- Reason for Murray's Law not being the optimum

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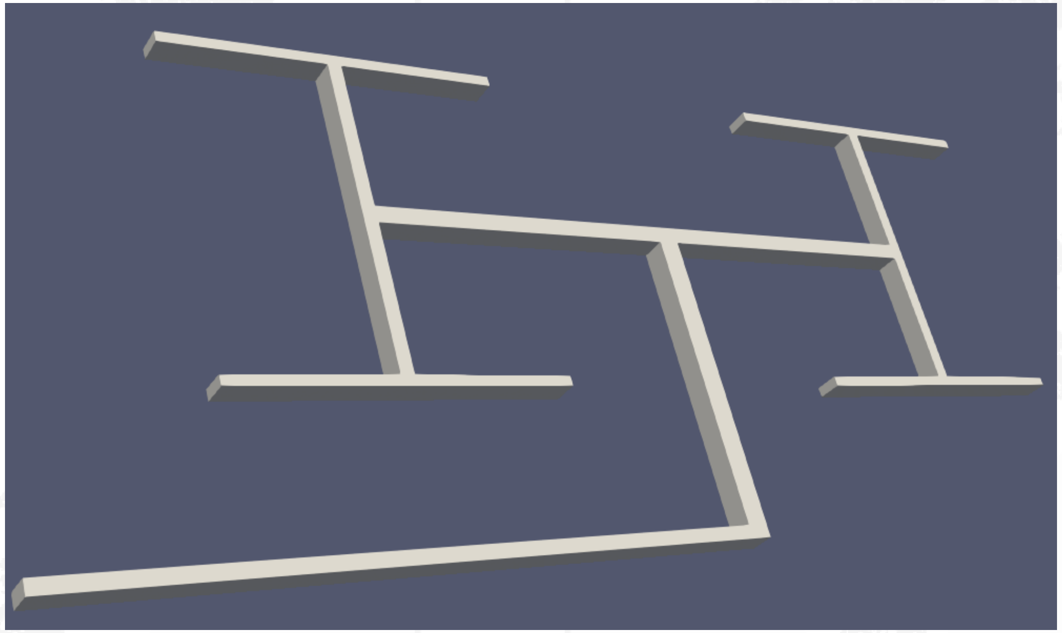
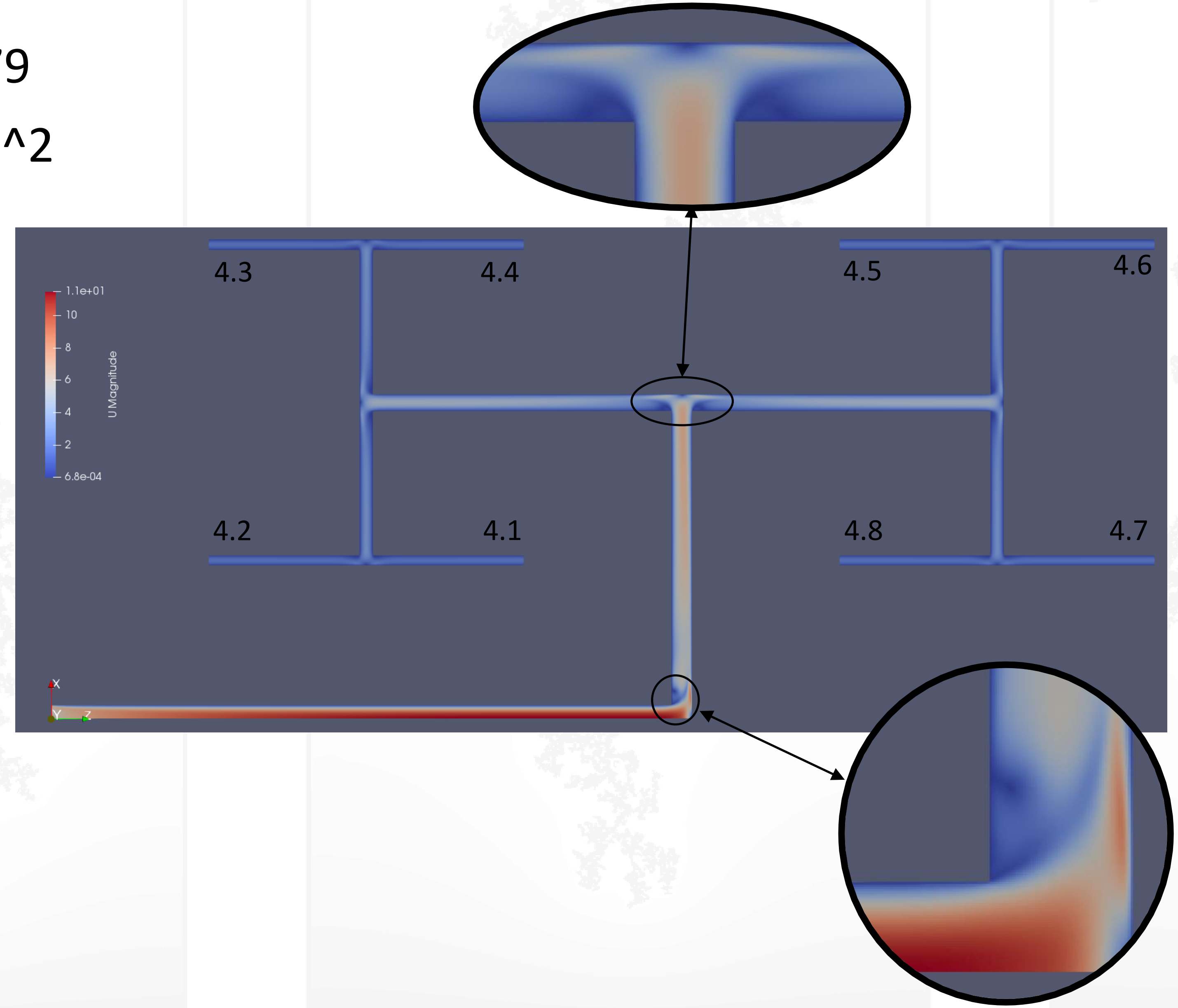
3D – Simulation setup

- Channel depth constant 1mm, channel width 1, 1.5, 2, 2.5 & 5mm
- *a* varied between 0.79, 0.9 and 1
- 4 generation levels
- Hexahedral mesh
- Incompressible, isothermal, laminar
- OpenFoam 4.1, simpleFoam

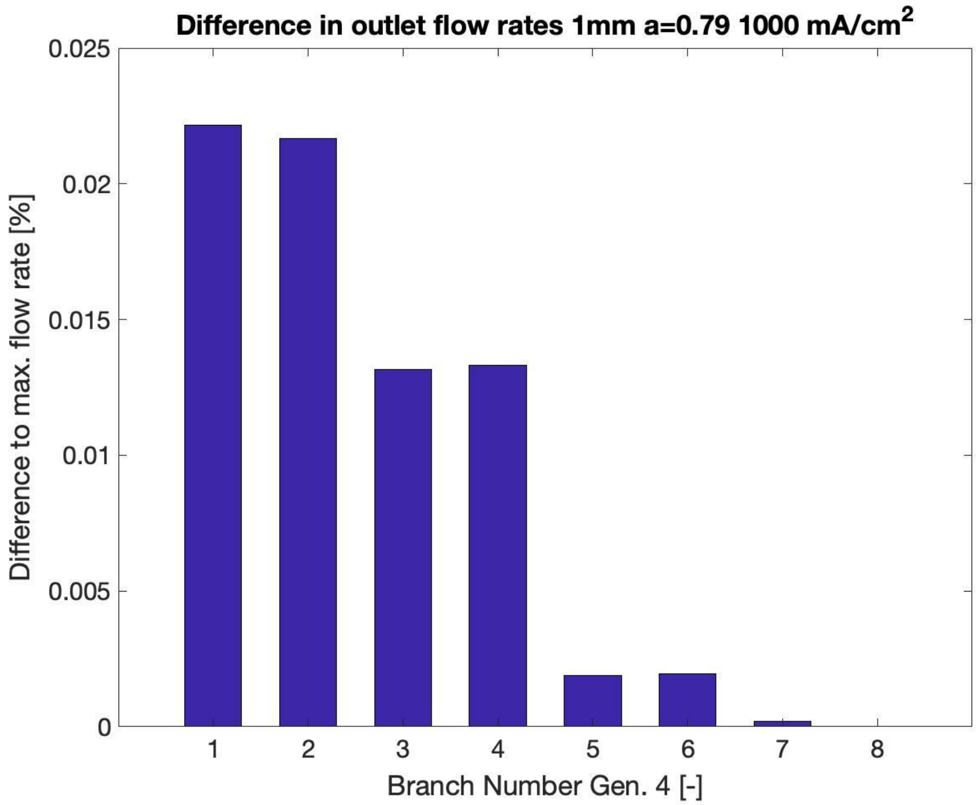


3D – Velocity & flow rate

- 1mm a=0.79
- 10000 A/m^2



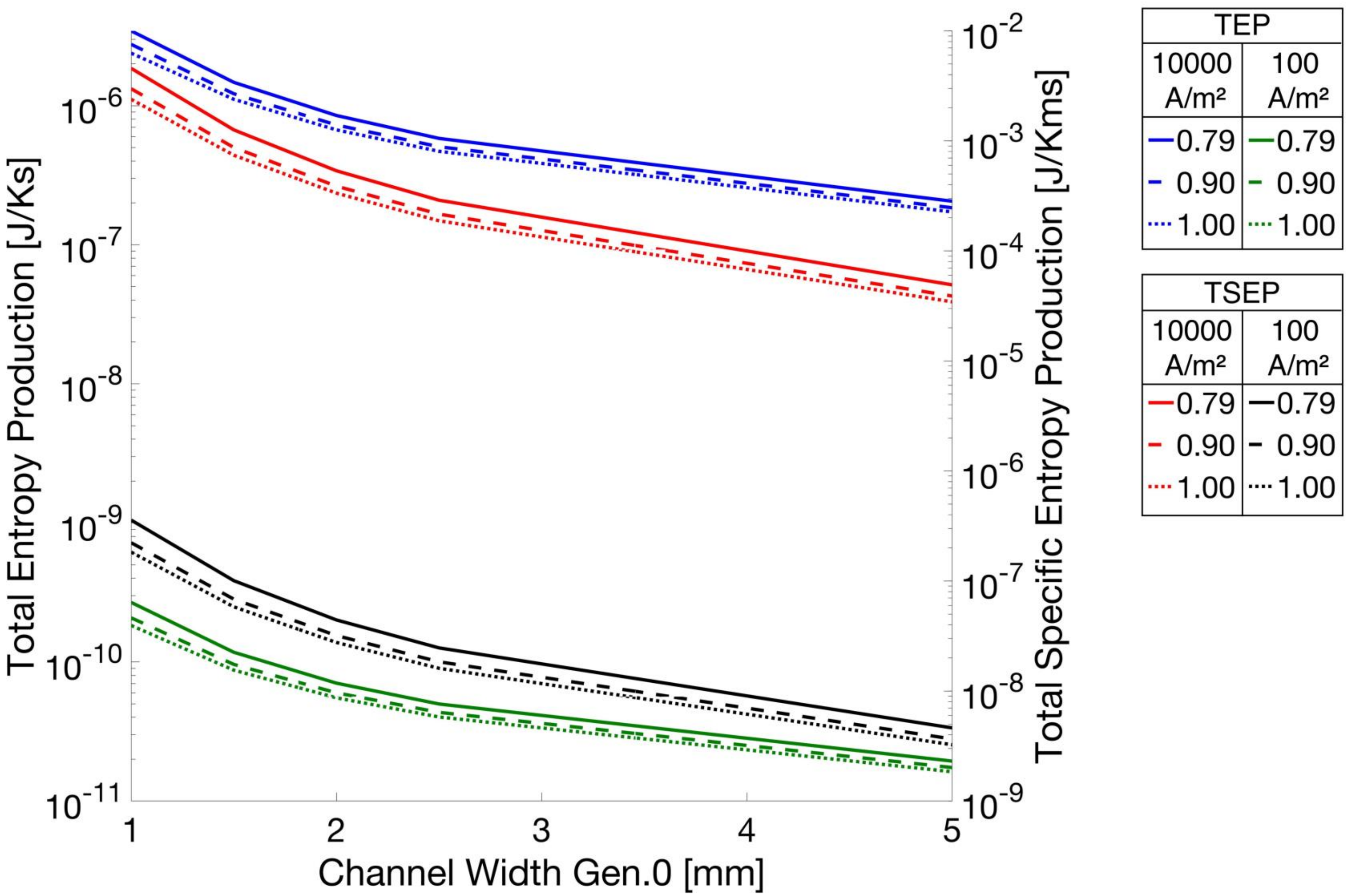
3D – Velocity & flow rate



	10000 A/m^2	5000 A/m^2	1000 A/m^2	100 A/m^2	10 A/m^2
w_0 =1mm, a =0.79	0.02	0.03	0.04	0.08	0.09
w_0 =1mm, a =0.9	0.11	0.20	0.27	0.53	0.56
w_0 =1mm, a =1	0.23	0.36	0.62	0.84	0.80
w_0 =1.5mm, a =0.79	0.03	0.01	0.01	0.01	0.01
w_0 =1.5mm, a =0.9	0.16	0.09	0.14	0.36	0.39
w_0 =1.5mm, a =1	0.37	0.14	0.17	0.46	0.47
w_0 =2mm, a =0.79	0.24	0.17	0.31	0.59	0.61
w_0 =2mm, a =0.9	0.29	0.03	0.04	0.09	0.09
w_0 =2mm, a =1	0.77	0.10	0.04	0.09	0.09
w_0 =2.5mm, a =0.79	0.20	0.02	0.03	0.06	0.07
w_0 =2.5mm, a =0.9	0.61	0.06	0.07	0.14	0.15
w_0 =2.5mm, a =1	0.75	0.11	0.18	0.34	0.37
w_0 =5mm, a =0.79	0.28	0.14	0.40	0.53	0.55
w_0 =5mm, a =0.9	2.54	0.41	0.70	0.90	0.91
w_0 =5mm, a =1	3.78	3.82	7.77	8.53	8.62

3D – Specific entropy production

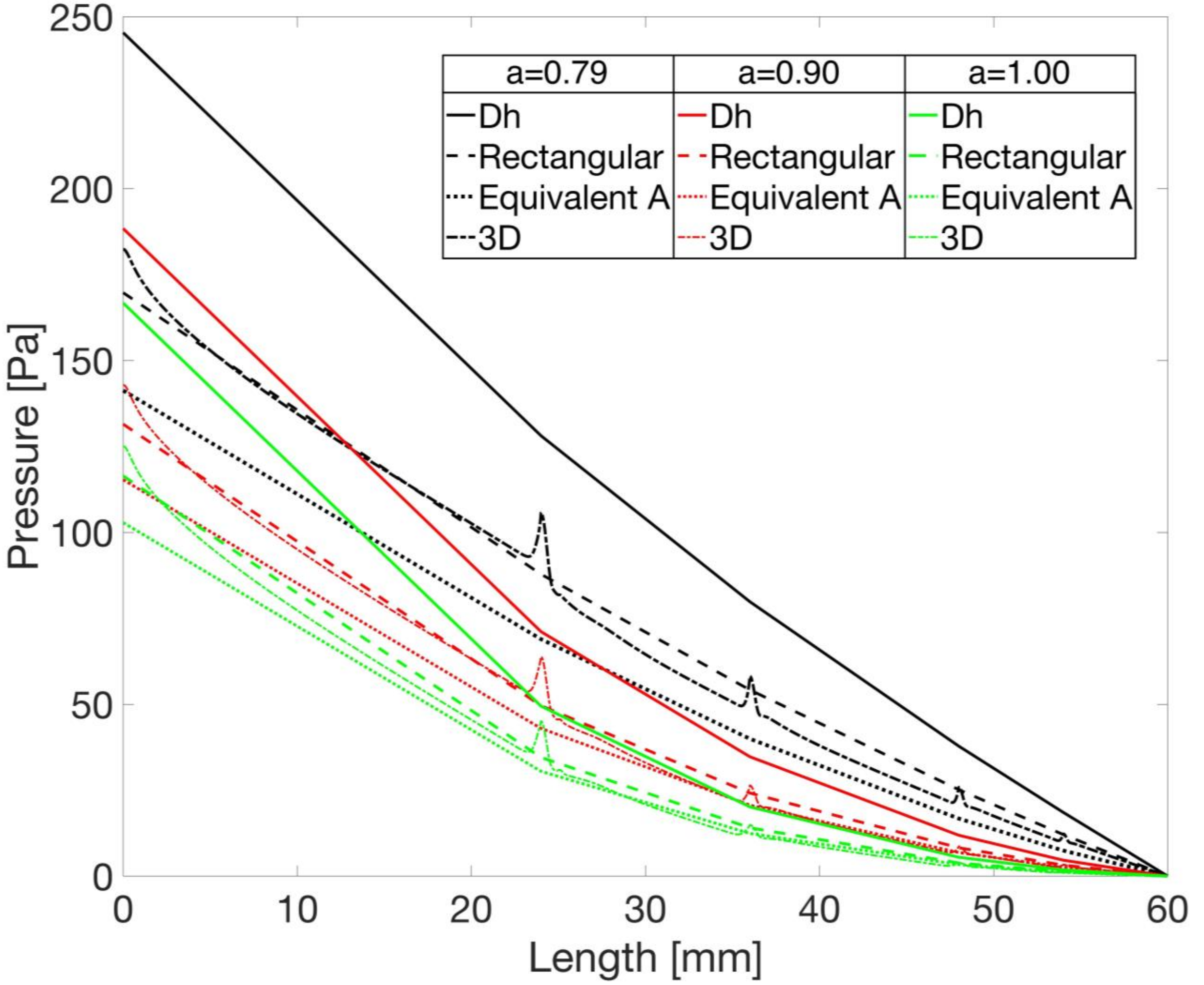
$$\left(\frac{dS_{irr_{specific}}}{dt}\right)_{j,i} = \left(\int_{V_{j,i}} -\frac{1}{T}\Pi : \nabla \boldsymbol{v} dV\right)\frac{1}{w_{j,i}} \qquad [5]$$



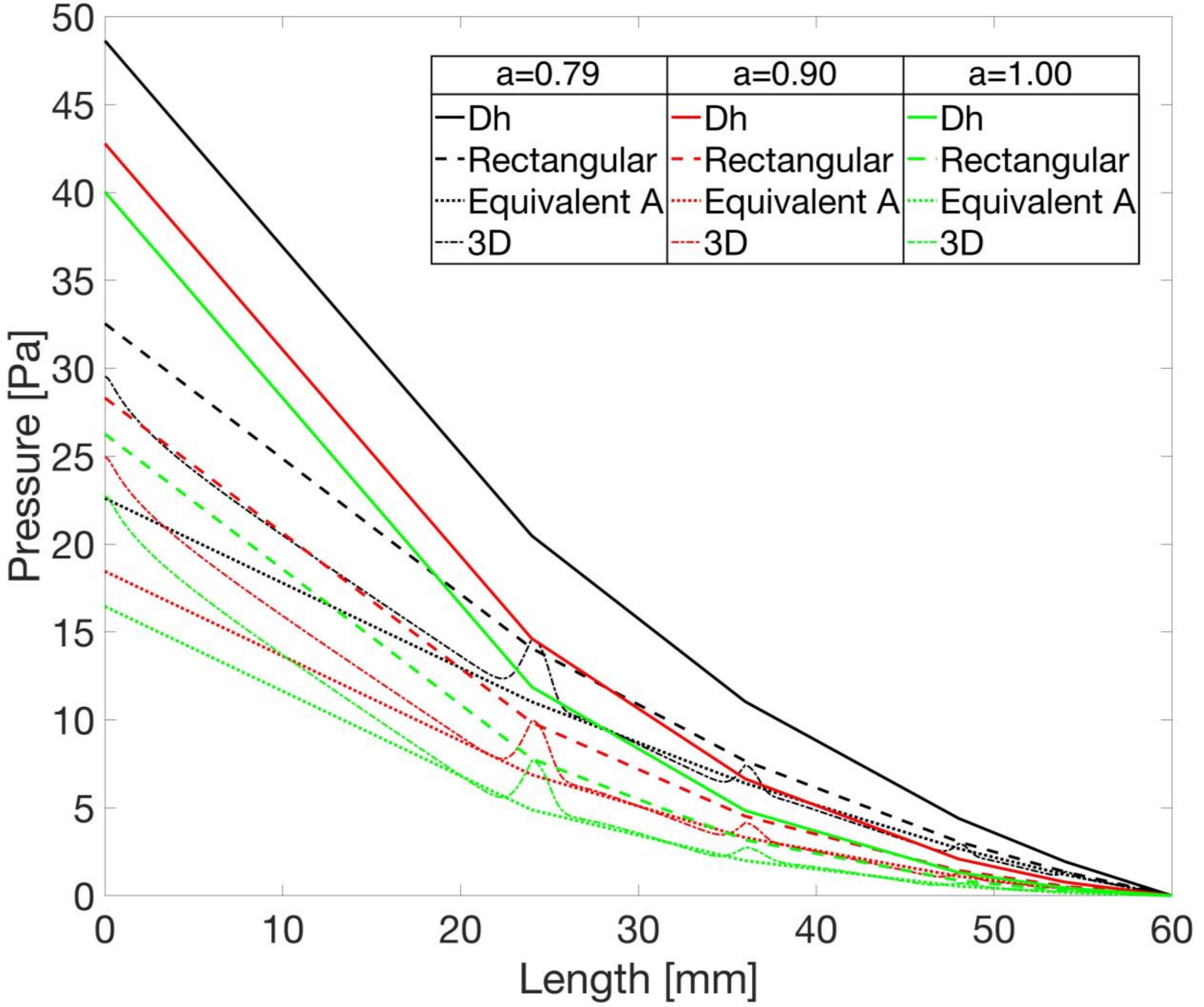
[5] S. Kjelstrup, D Bedeaux, E. Johannessen and J. Gross. Non-Equilibrium Thermodynamics for Engineers. World Scientific, 2 edition, 2017.

3D - Pressure

w_0=1mm



w_0=2.5mm



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3D – Summary

- Uniform flow distribution (beside w_0=5mm cases)
- Results give same conclusions than for the 1D calculations
  - Murray's Law does not deliver the lowest entropy production
  - Increase in width → decrease in entropy production
- Most exact pressure drop calculation method depends on channel shape

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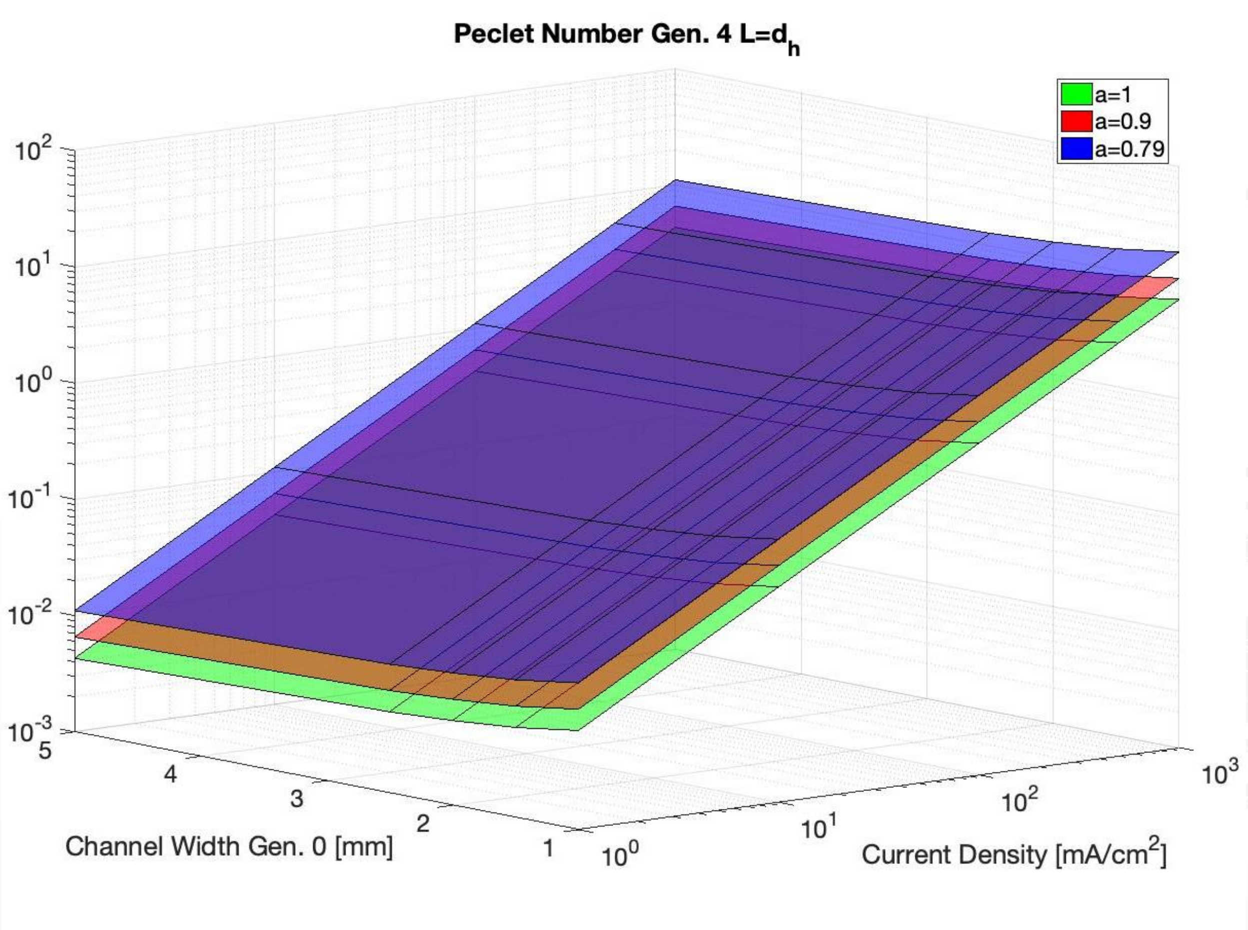
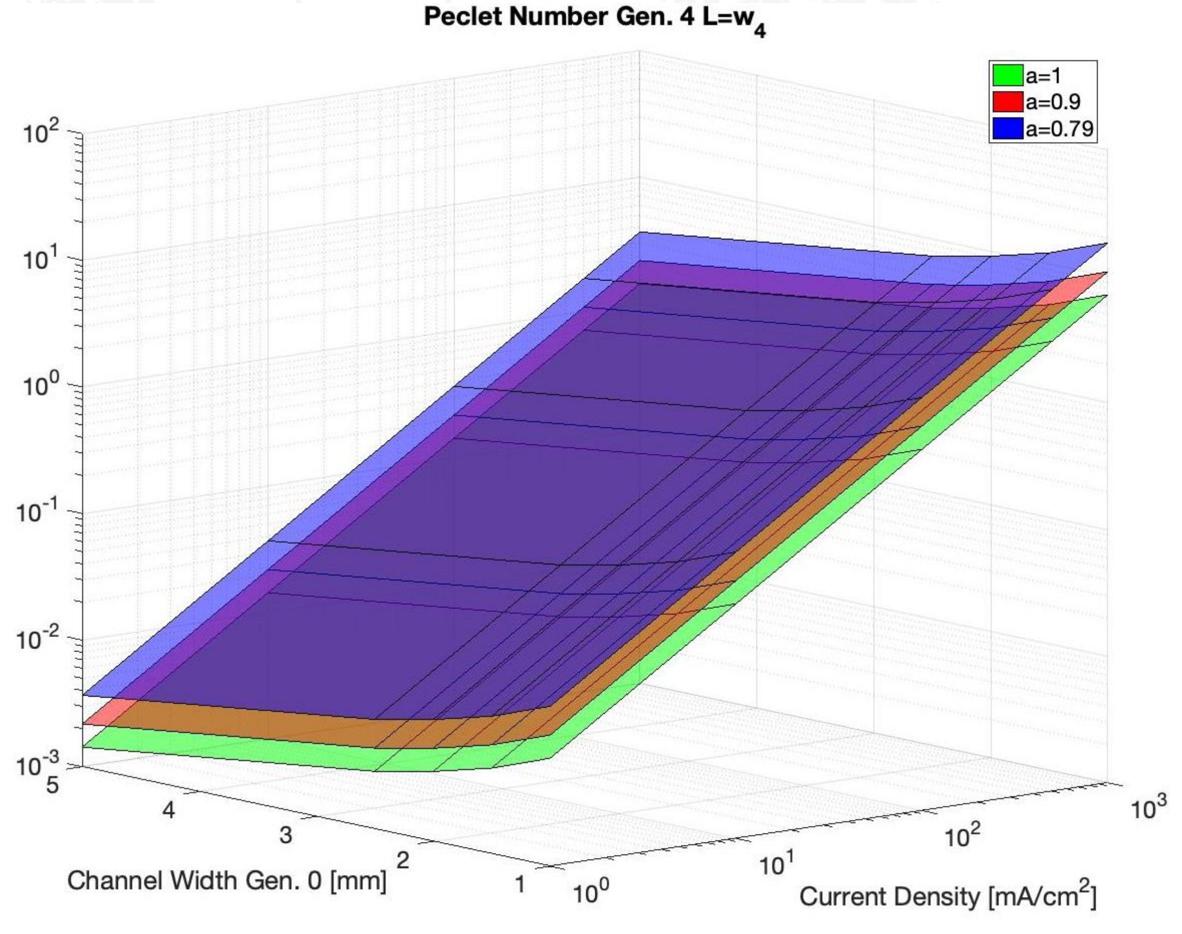
Peclet number

$$Pe = \frac{Lv}{D}$$





Discussion

- Due to uniform flow distribution, PEMFC can be subdivided
- Allows for approximation with 1D model

- Advantages of this pattern:
  - Easy to change space filling properties
  - Increase in generation levels does not increase pressure drop significantly (a>0.79)
  - This is due to the scaling

- Compared to serpentine:
  - Lower pressure drops achieveable (1 order of magnitude) [6]
  - Uniform fuel distribution

- Not only applicable for PEMFCs, but also other fuel cells

[6] Su, A., Chiu, Y. C., and Weng, F. B. (2005). The impact of flow field pattern on concentration and performance in pemfc. *International Journal of Energy Research*, 29(5):409–425.

Conclusions

- Tree-shaped pattern provides uniform velocity/flow rate at end of last branches
- The higher the *a*, the lower the entropy production
- Scaling parameter *a* acc. to Murray's Law not optimal
- To use the hydraulic diameter approximation, overestimates the pressure drop and EP.
- The best way depends on the channel shape
- The Peclet number analysis gives a range of current densities where Pe<1 can be achieved

Thank you for your attention!

Any questions?

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We gratefully acknowledge the support from NTNU in Trondheim and the Research Council of Norway through its Centre of Excellence funding scheme with Project No. 262644 (PoreLab) and UNINETT Sigma2 - the National Infrastructure for High Performance Computing and Data Storage in Norway