

Metasurface-Engineered Anode for Solid Oxide Electrolysis Cells

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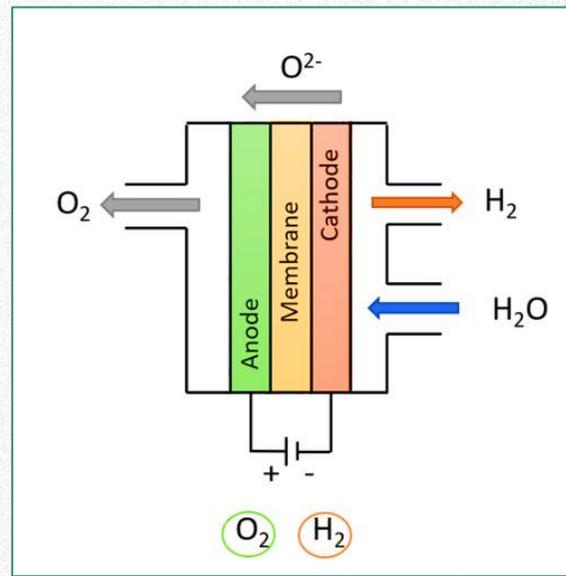
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Introduction

Uses of H₂?

- **For propulsion**
- Refining petroleum
- Treating metal
- Producing fertiliser
- Processing foods
- Energy storage and producing electricity for a wide variety of devices and vehicles
- Burning hydrogen blended with natural gas



Solid oxide electrolysis cell (SOEC)

For steam electrolysis:



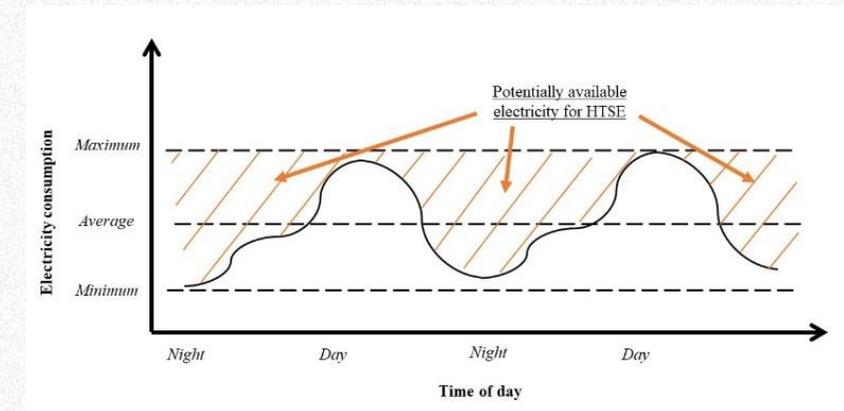
For carbon dioxide electrolysis:



Uses of O₂?

- **Breathable air for life support systems (Hoffman et al., 2023)**
- As oxidizer, for propulsion, welding, cutting
- For medical applications

SOEC is suitable for intermittent energy consumption and operation



Introduction

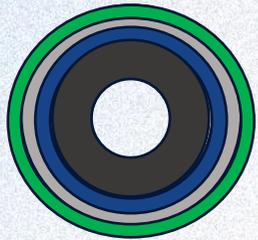
Current challenges

1. **Costs.**
2. Material degradation.
3. Fabrication of cells.
4. Lack of commercialization.

Advantages

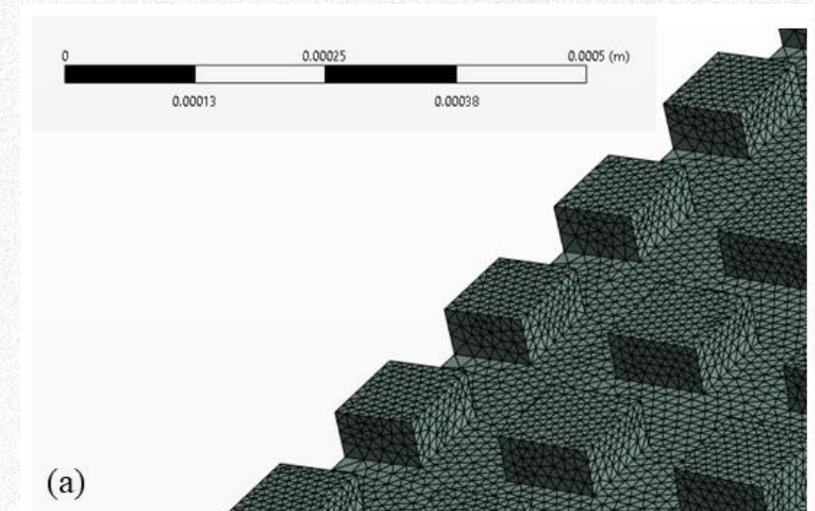
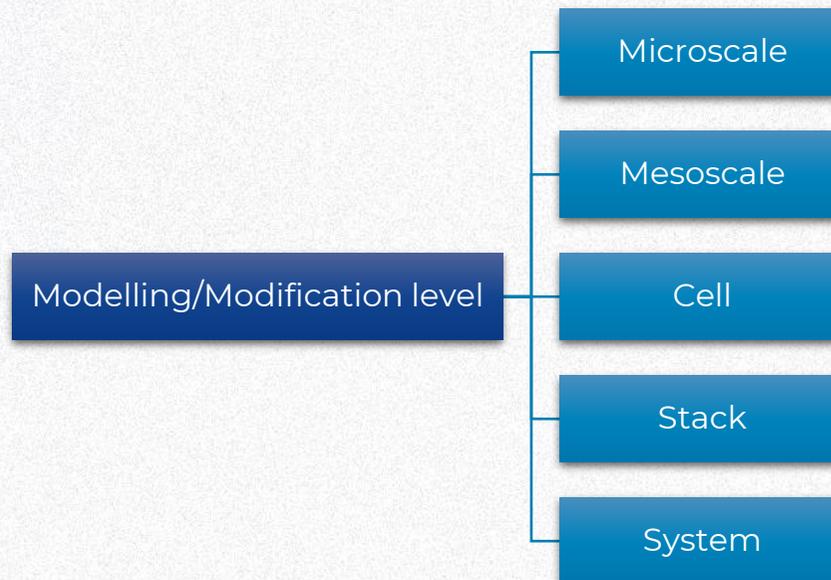
1. **High efficiency.**
2. Compatibility with a wide range of systems.
3. Intermittent operation.
4. Use of solid materials.
5. Environmentally friendly.
6. Produced gases are free from contaminants.

Metal-supported cell



+ High mechanical stability

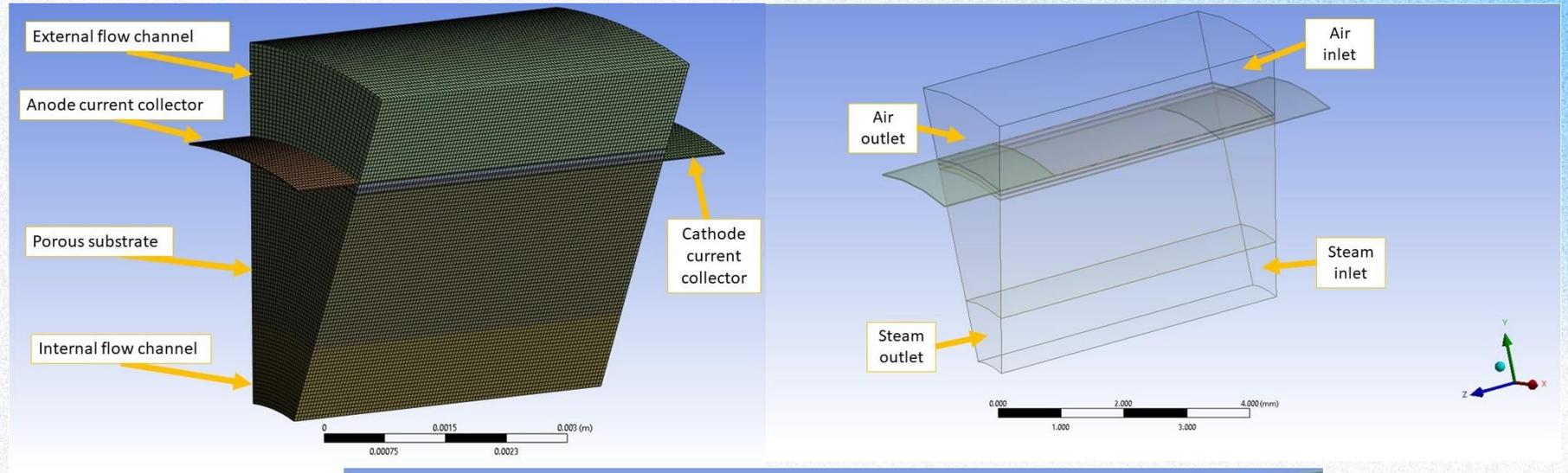
- Energy losses in the supporting porous metal layer



Computational fluid dynamics (CFD) model: Baseline model

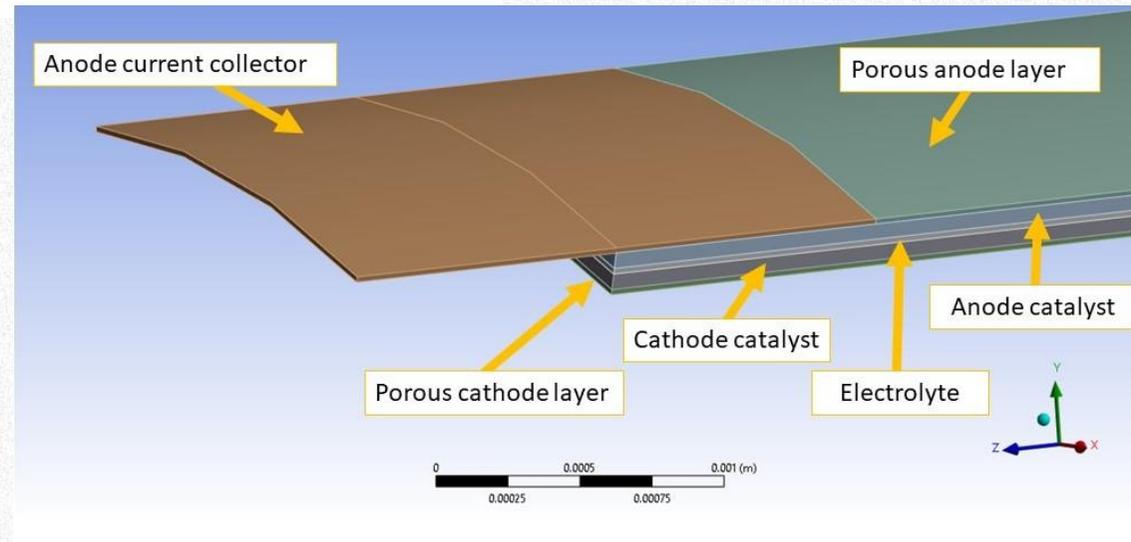
Boundary conditions:

- 2 Inlets
- 2 Outlets
- Remaining boundaries are assumed to be Walls



ANSYS 2023 R1 resolved electrolyte simulations:

- Continuity equation
- Momentum balance (laminar flow model)
- Species transport
- Electrochemistry



Computational fluid dynamics (CFD) model: Baseline model

SOEC sizes and materials

Structure	Internal diameter, mm	Wall thickness, mm	Materials	Volume proportion	Design porosity, %
Substrate	6.00	2.15	Ti	100%	30
Cathode current collector	10.30	0.02	Ag	100%	0
Porous cathode	10.30	0.02	NiO, GDC	60%:40%	30
Cathode	10.34	0.06	NiO, GDC	60%:40%	30
Electrolyte	10.46	0.022	GDC, YSZ	91%:9%	30
Anode	10.504	0.06	GDC, LSCF	50%:50%	30
Porous anode	10.624	0.02	GDC, LSCF	50%:50%	30
Anode current collector	10.624	0.02	Ag	100%	0

Material properties

Material composition of the layer	Density, kg/m ³	Specific heat, J/(kg*K)	Thermal conductivity, W/(m*K)	Electrical conductivity calculated/Referenced, S/m
Titanium	4850	544	7	2381000
Silver	10490	235	429	6300000
Nickel	6670	445	91	25000
LSCF	6000	340	58	6
YSZ	5900	620	2	2
GDC	7200	216	11	99

Properties of layers composed of material mixtures

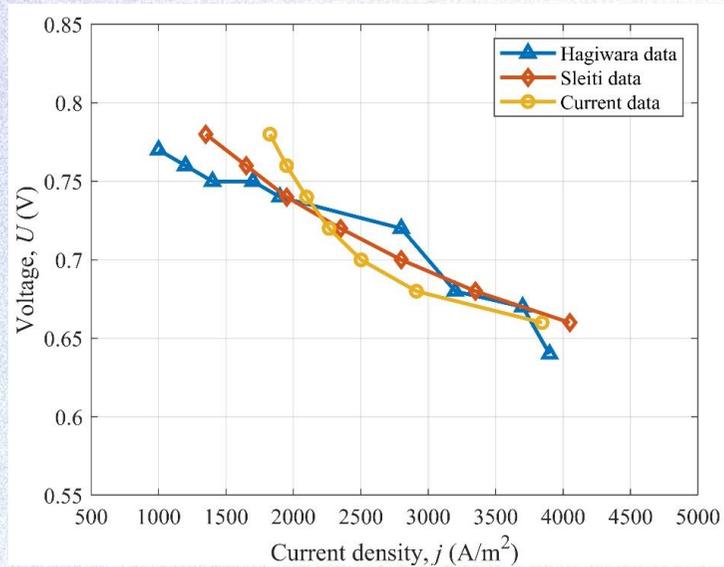
Material composition of the layer	Proportion of materials	Density, kg/m ³	Specific heat, J/(kg*K)	Thermal conductivity, W/(m*K)	Electrical conductivity calculated/Referenced, S/m	Default suggested electrical conductivity, S/m	Function of the layer
NiO, GDC	60%:40%	6882	353	59	15040	5000	Cathode
GDC, YSZ	91%:9%	7083	252	10	91	1e-16	Electrolyte
GDC, LSCF	50%:50%	6600	278	35	53	5000	Anode

Operating conditions

Parameter, units	Value
Temperature, K	1073
Steam inlet mass flow rate, kg/s	1e-5
Air inlet mass flow rate, kg/s	1e-6
Pressure, Pa	Atmospheric

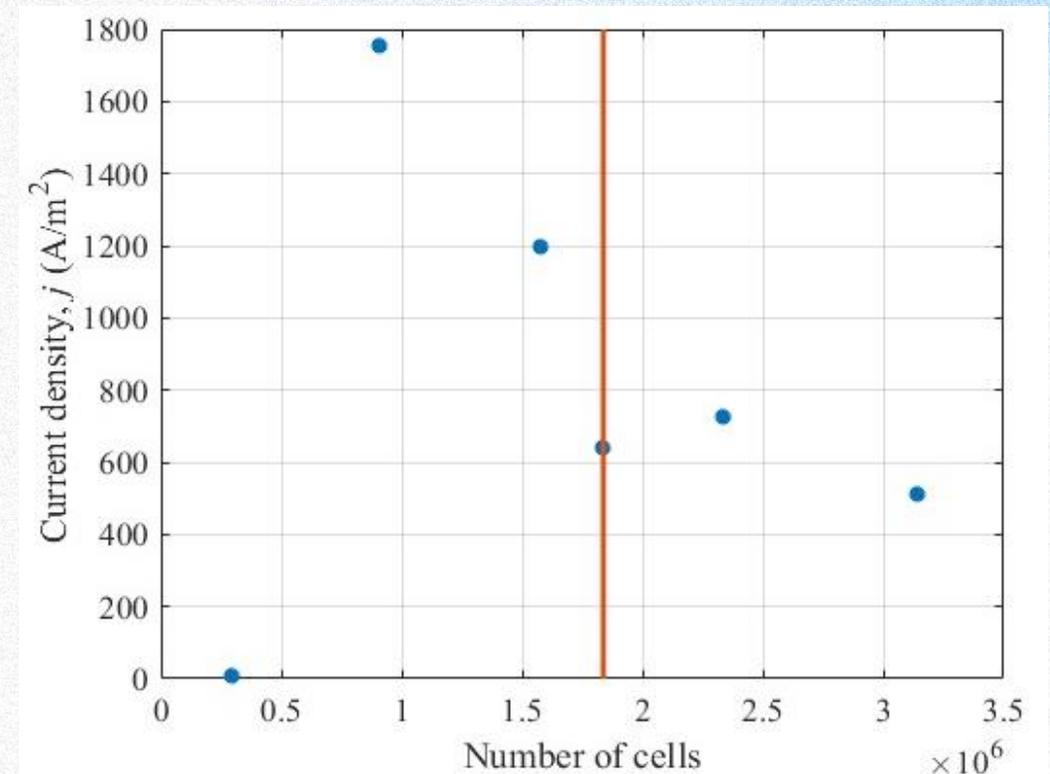
Computational fluid dynamics (CFD) model: Verification and validation

Validation with the data by Sleiti (2010)



Mesh number	Cell count	Element size, m	Current density, A/m^2
Mesh 1	93 852	0.00055	6 679
Mesh 2	213 516	0.00040	5 579
Mesh 3	609 356	0.00027	3 707
Mesh 4	648 000	0.00026	2 463
Mesh 5	713 440	0.00025	2 953
Mesh 6	928 806	0.00023	2 576

Mesh independence test for 1.5V



ANALYSIS I: Study of rectangular shaped metasurface elements

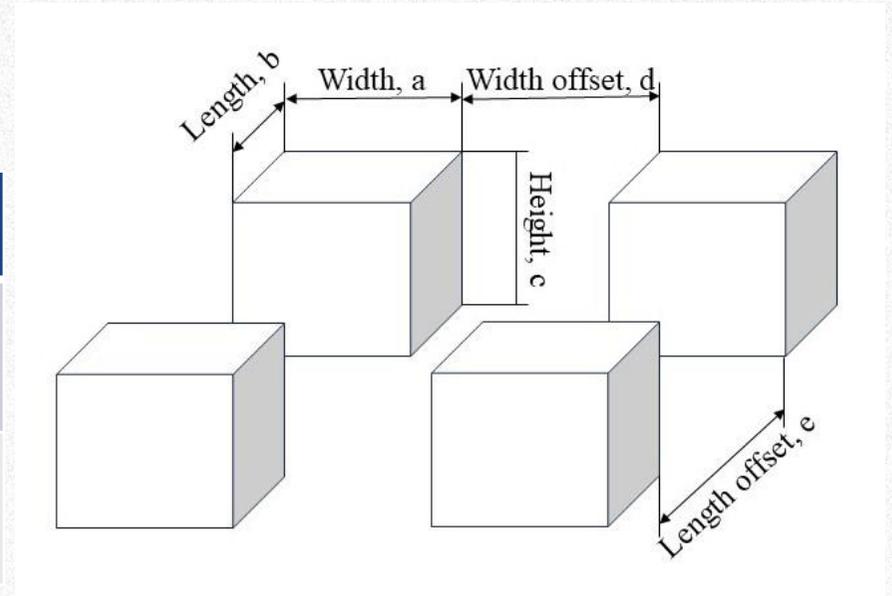
Research question / aim 1:

Identify an optimal size of rectangular shaped elements of the anode metasurface.

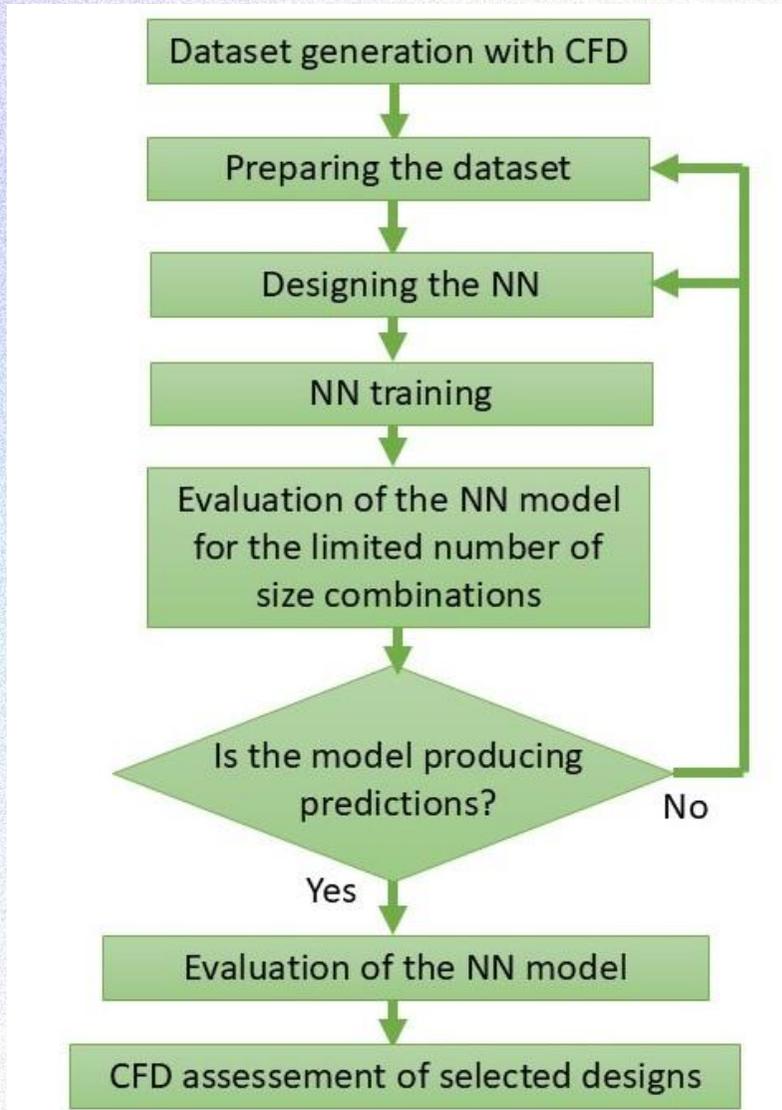
Research objectives:

1. Build the neural network model of the current density for SOEC with metasurfaces for the range of element sizes.
2. Evaluate the current density for all range of sizes.
3. Identify the optimal size of a metasurface element by the highest current density.

Sizes of rectangular shaped metasurface elements	Optimization limits
Length b , height c , distance between the elements along the length of the tubular cell (length offset) e	From 0.025 mm to 0.6 mm
Width a , distance between the elements along the circumference of the tubular cell (width offset) d	From 0.2675 degrees to 6.42 degrees



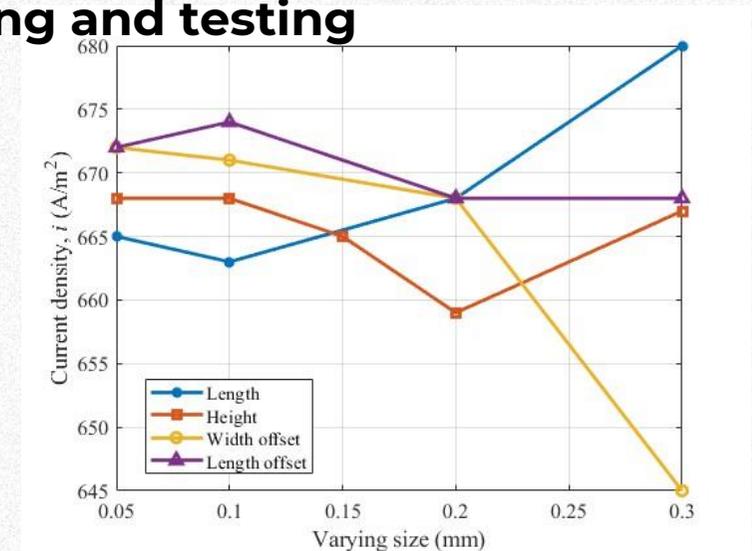
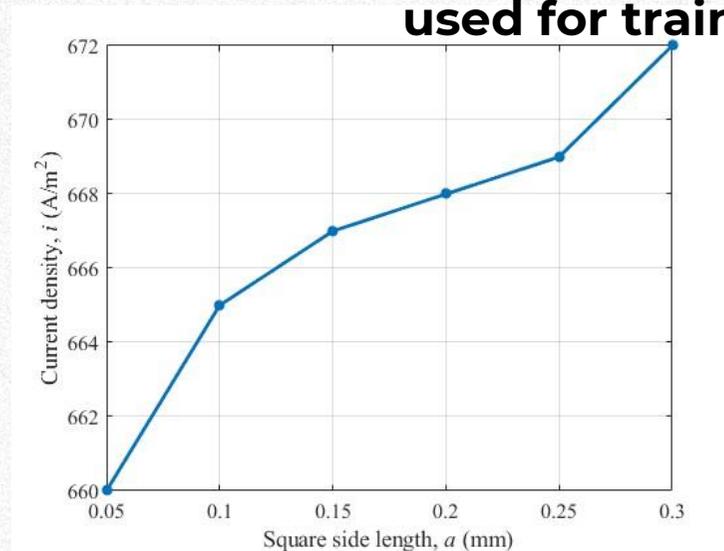
ANALYSIS I: Study of rectangular shaped metasurface elements



Final ANN architecture

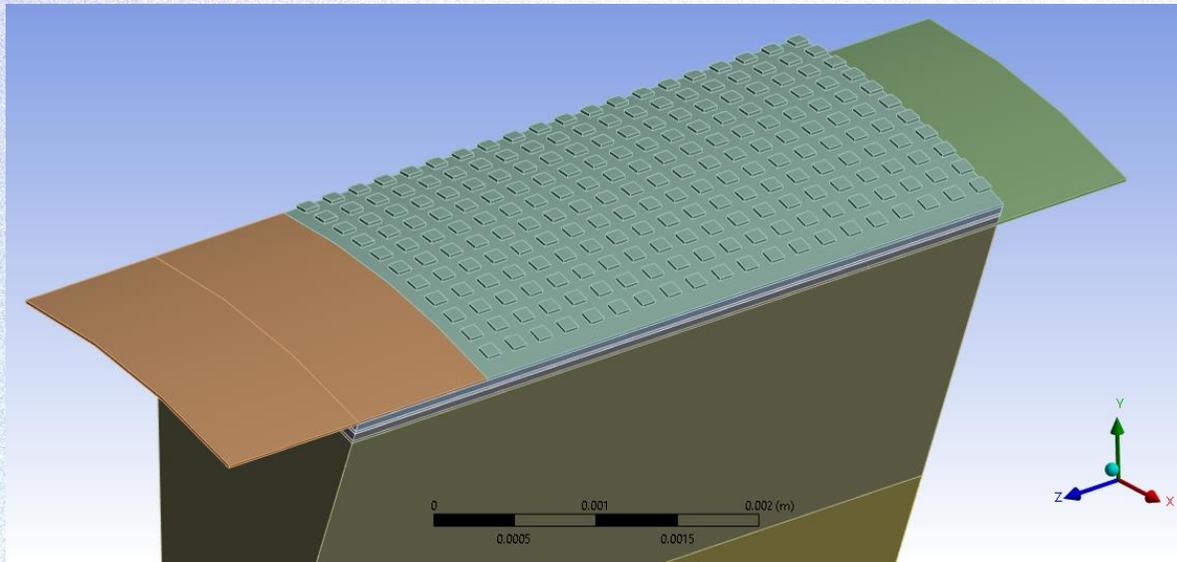
Layer #	Number of neurons	Activation function
1	5	Linear
2	8	Sigmoid
3	16	Sigmoid
4	32	Sigmoid
5	16	Softplus
6	8	ReLU
7	4	ReLU
8	1	Linear

Patterns in the CFD dataset for 1.5 V used for training and testing

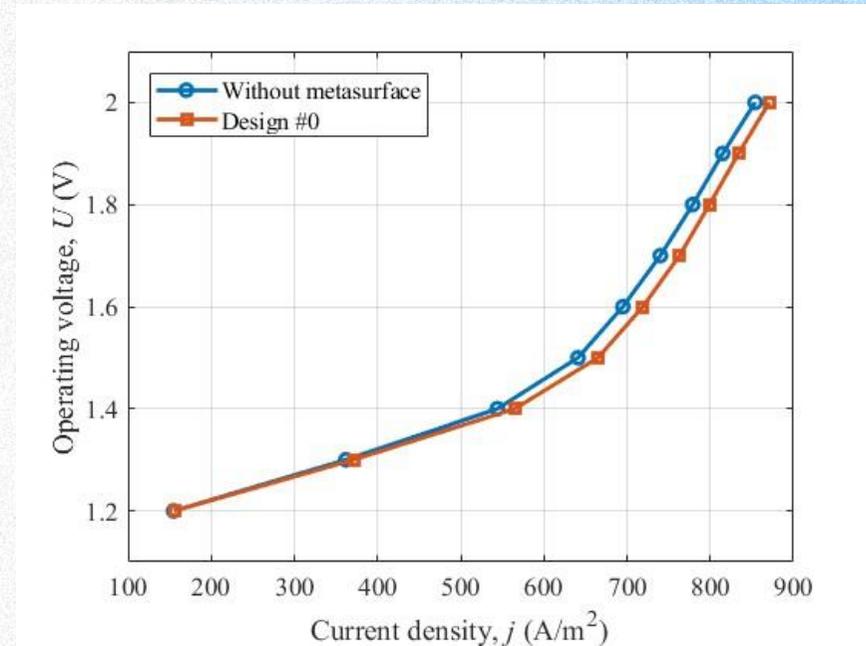


ANALYSIS I: Study of rectangular shaped metasurface elements

Design #0 metasurface



Comparison of Design #0 and no metasurface



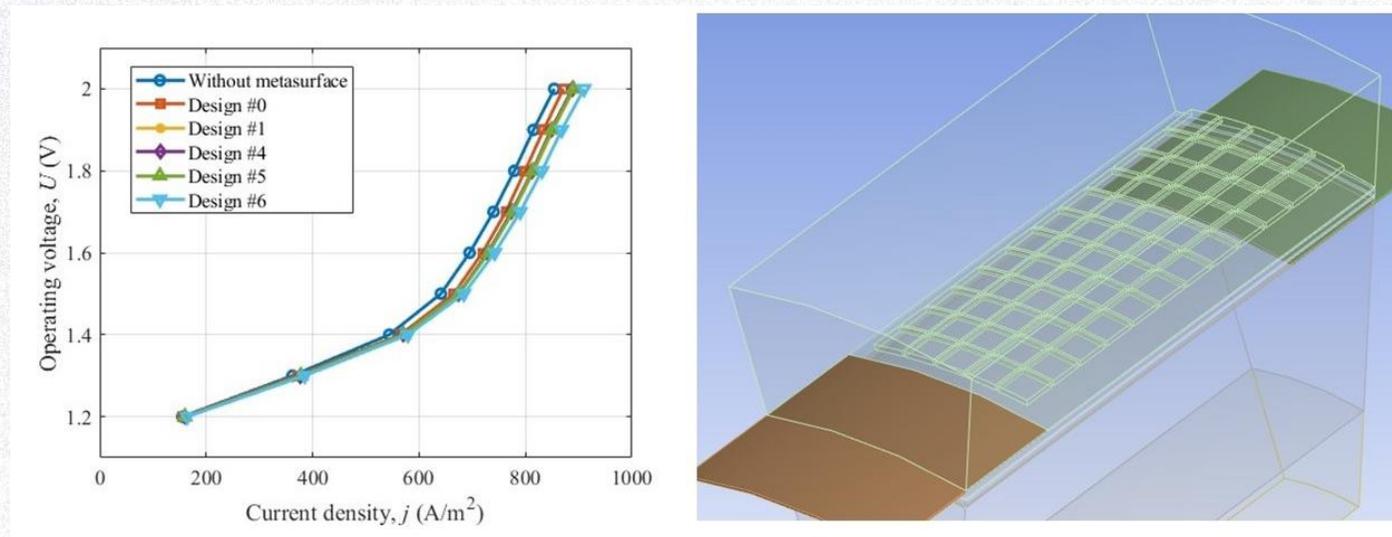
Example of points included in the dataset for 1.5 V

Design #	Width, deg	Length, mm	Height, mm	Width offset, deg	Length offset, mm	NN-predicted current density, A/m ²	CFD-predicted current density, A/m ²	Improvement in current density compared to No metasurface
No metasurface							641	-
0	1.07	0.1	0.050	1.07	0.100	Included in dataset	665	3.7%

ANALYSIS I: Study of rectangular shaped metasurface elements

Top 6 size combinations from 497 616 size combinations evaluated

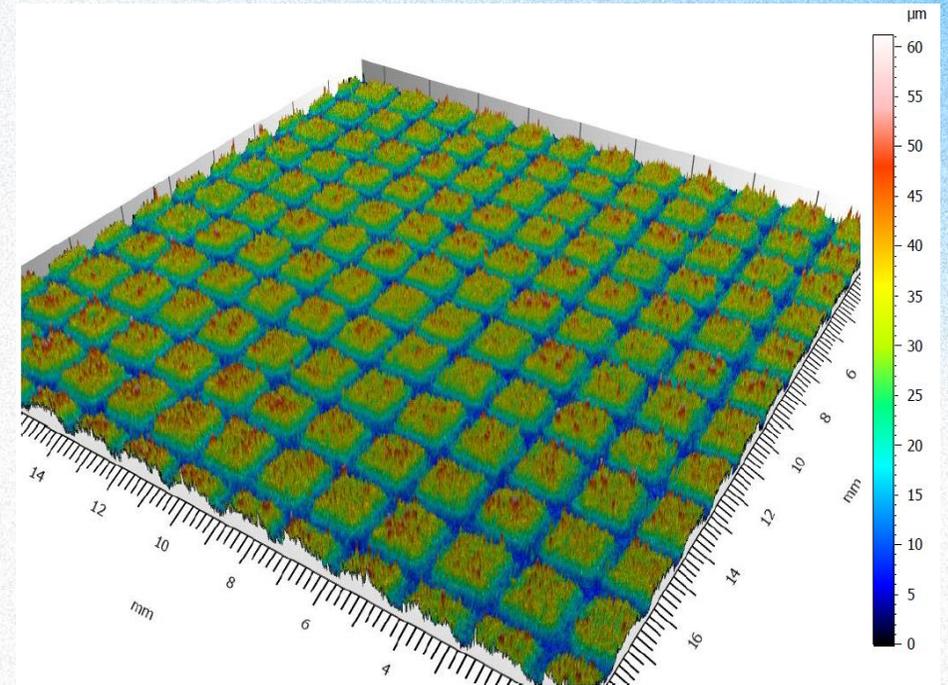
Design #	Width, deg	Length, mm	Height, mm	Width offset, deg	Length offset, mm	NN-predicted current density, A/m ²	CFD-predicted current density, A/m ²	Improvement in current density compared to no metasurface
No metasurface							641	-
0 (Small squares)	1.07	0.1	0.050	1.07	0.100	Included in dataset	665	3.7%
1	6.42	0.3	0.025	2.14	0.025	675.68	675.43	5.4%
2	6.42	0.3	0.025	1.8725	0.025	675.68	673.99	5.1%
3	6.42	0.3	0.025	2.4075	0.025	675.68	672.24	4.9%
4	3.21	0.3	0.025	0.2675	0.025	675.33	673.72	5.1%
5	3.21	0.3	0.025	0.535	0.025	675.31	674.59	5.2%
6	3.21	0.3	0.05	0.2675	0.025	675.30	684.12	6.7%



ANALYSIS I: Study of rectangular shaped metasurface elements

Conclusions from Analysis I:

- ❑ CFD dataset of 51 combinations of element sizes with respective current density levels created.
- ❑ ANN model is built, trained and checked to predict the current density characteristics based on the combination of 5 sizes of rectangular shaped metasurface elements.
- ❑ 497 616 combinations of sizes are evaluated by the trained ANN model and ranked by the level of the current density.
- ❑ Top 6 designs are checked with the CFD analysis.
- ❑ The most efficient metasurface has the 6.7% increase in the current density characteristics at 1.5 V compared to the case without metasurface.



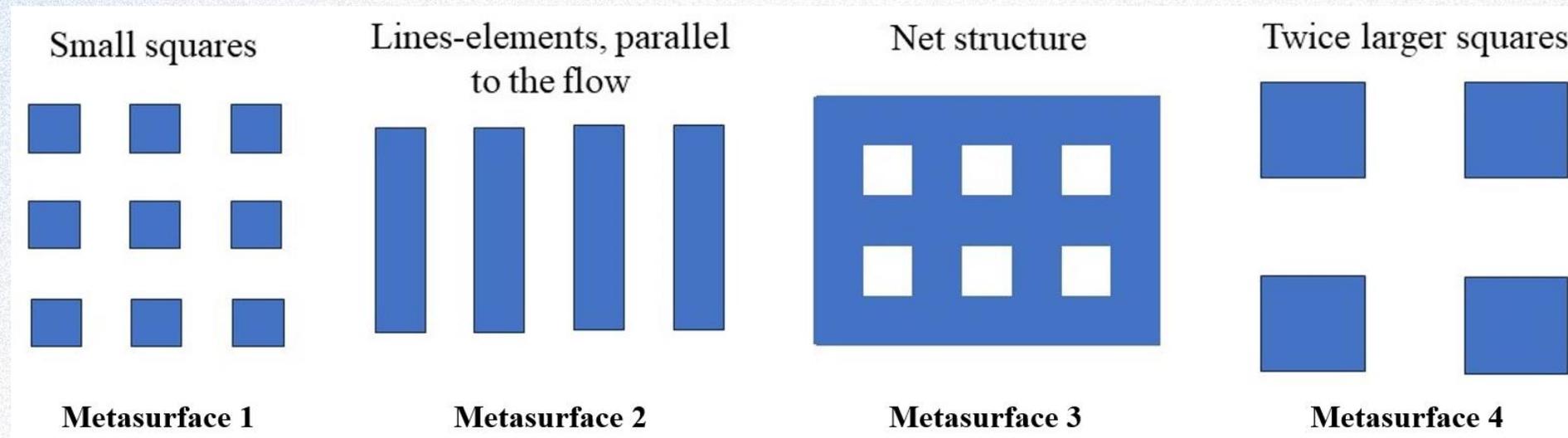
ANALYSIS II: Study of different regular metasurface patterns

Research question / aim 2:

Identify an optimal type of geometrical shape for anode metasurface elements.

Research objectives:

1. Conduct CFD simulations for four metasurface patterns to evaluate the current density.
2. Identify the most efficient metasurface pattern.
3. Investigate the fluid dynamics mechanism behind the efficiency of metasurface patterns.



ANALYSIS II: Study of different regular metasurface patterns

Metasurface options' characteristics for selected voltage

#	Metasurface types	No. of metasurface elements	No. of mesh cells	No. of iterations	Current density*, A/m ²	Current density **, A/m ²	Current density ***, A/m ²
0	Without metasurface (Base case)	0	1 837 632	1000	641	647	476
1	Small squares	11 x 20 square elements	5 028 880	200	665	668	492
2	Lines, parallel to the flow	11 line-elements	5 558 873	200	690	691	510
3	Net structure	11 x 20 line-elements	5 938 371	200	696	698	512
4	Large squares	5.5 x 10 square elements	4 636 929	200	668	670	493

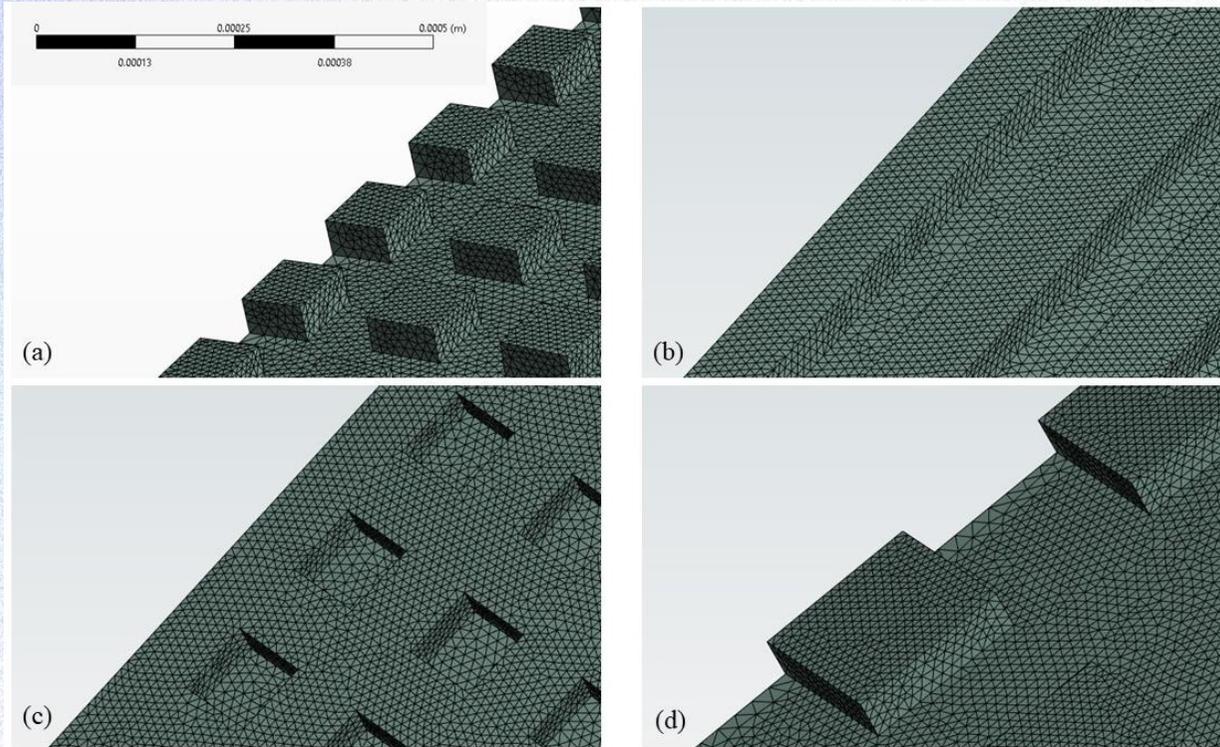
*** At 1.5V operating voltage & the OCV of 1.1 V**

**** At 1.8V operating voltage & the OCV of 1.4 V**

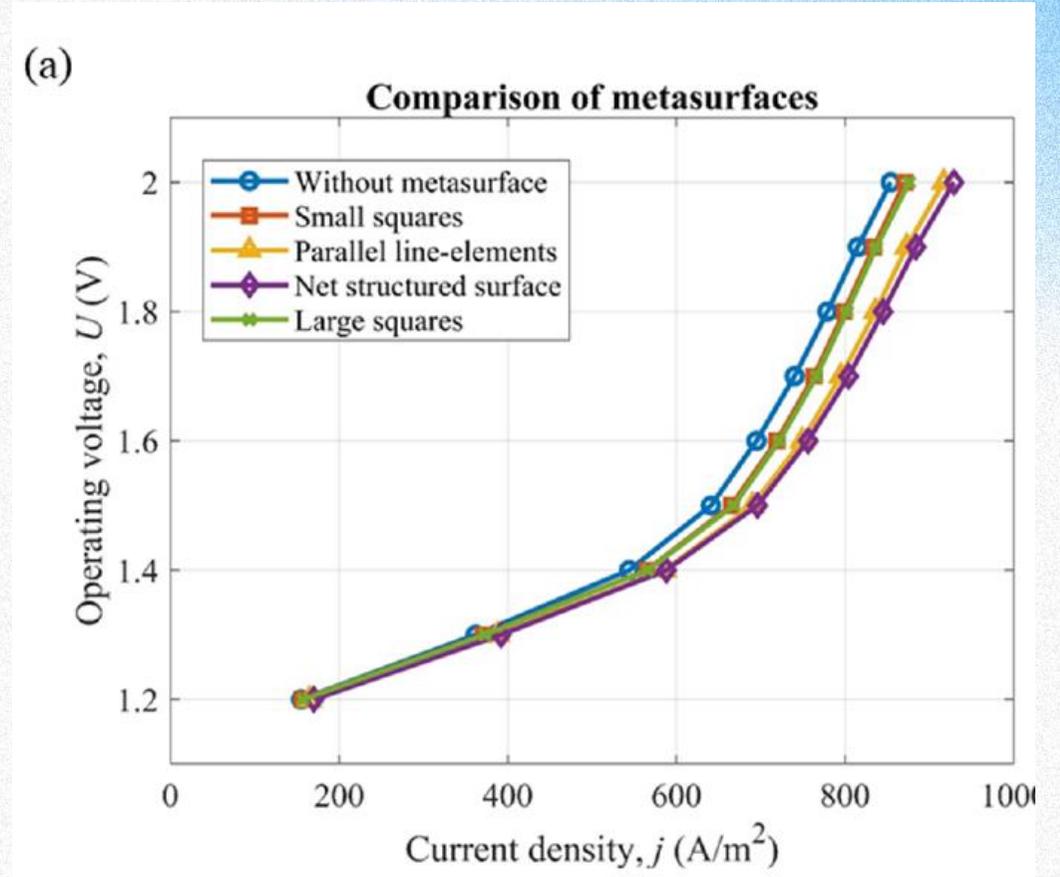
***** At 1.1V operating voltage & the OCV of 0.84 V**

ANALYSIS II: Study of different regular metasurface patterns

Meshed anode metasurface options

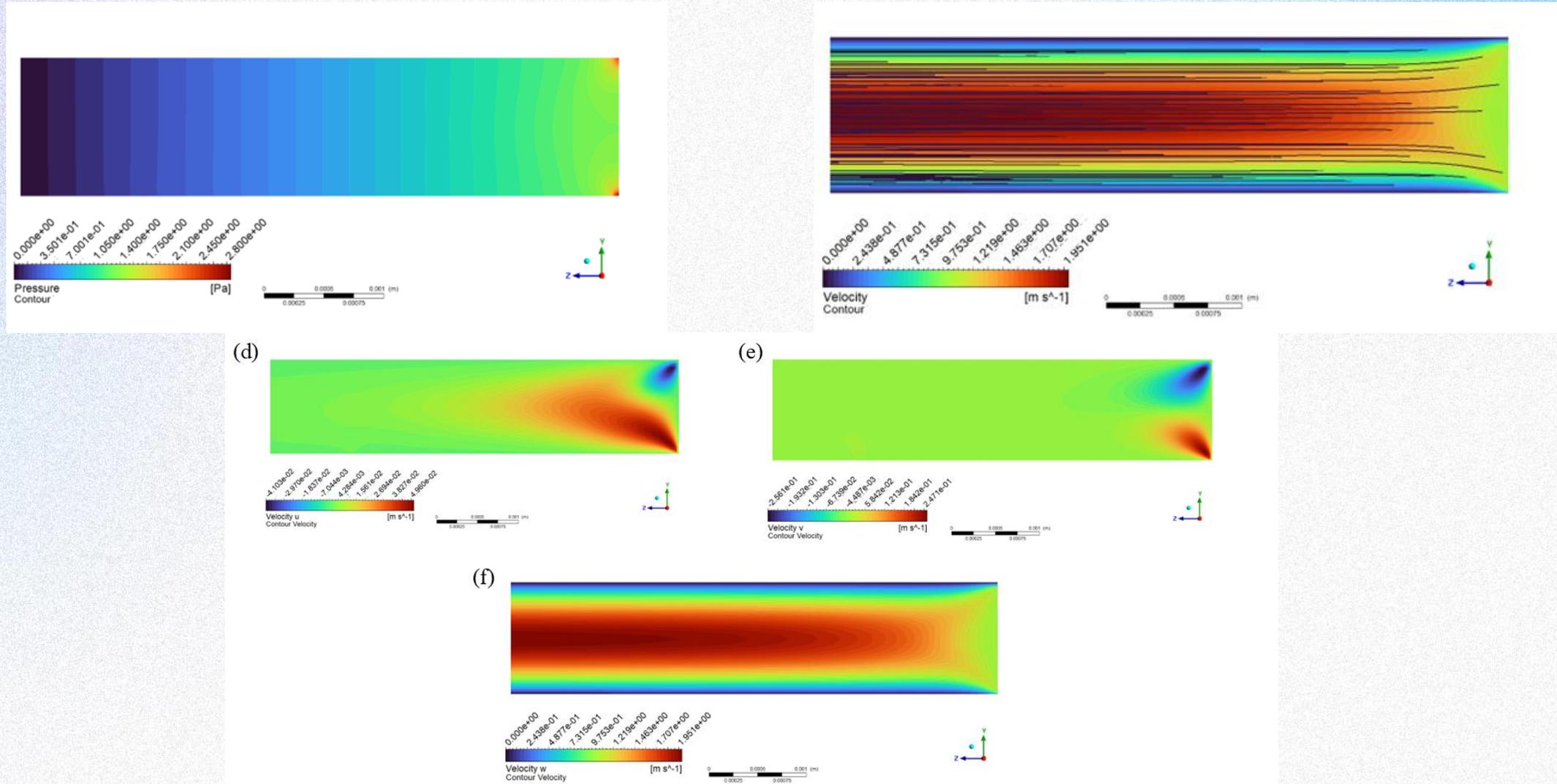


Full voltage – current density characteristics



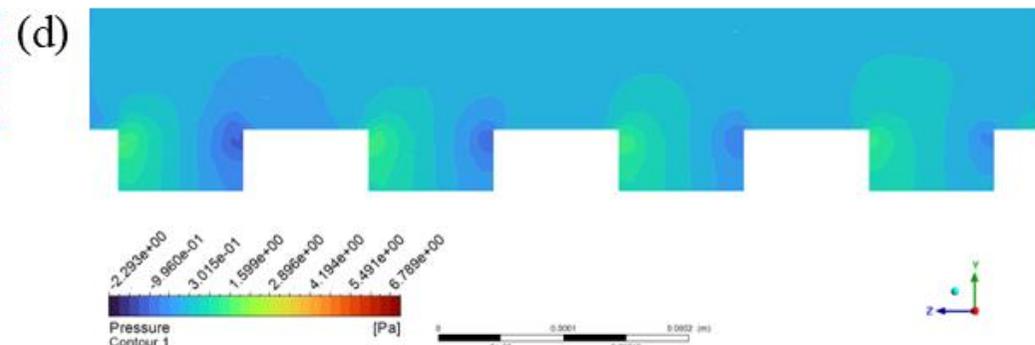
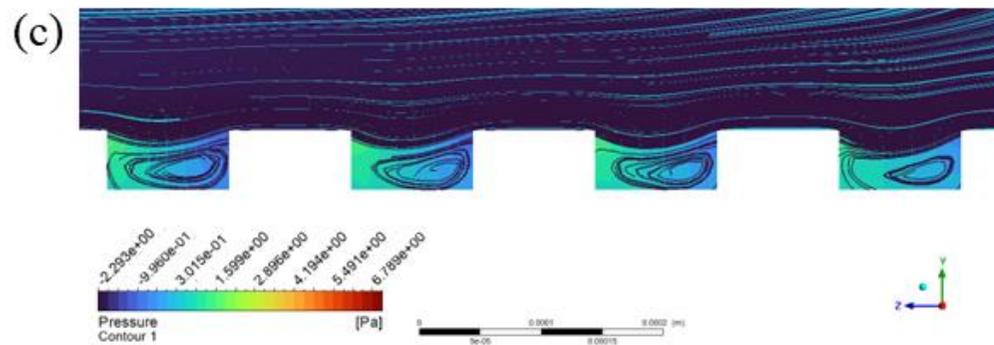
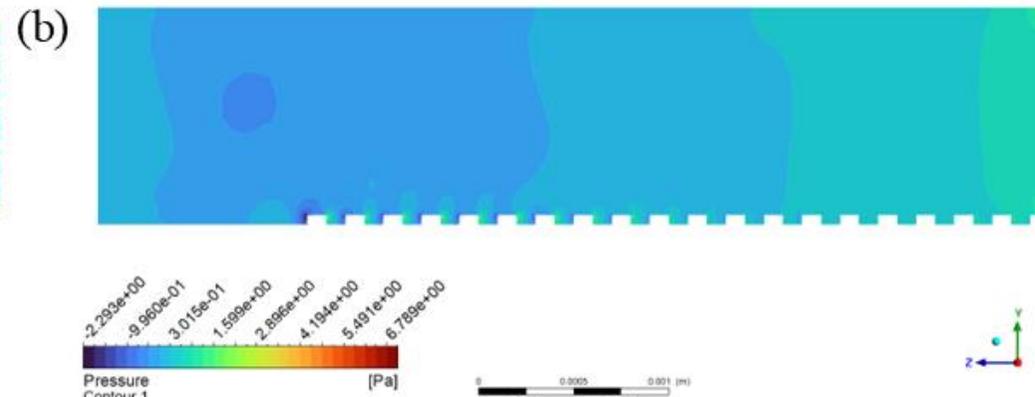
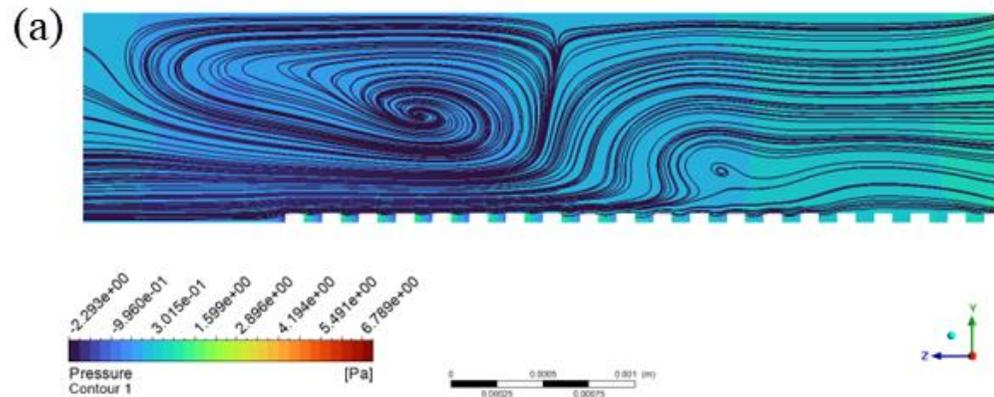
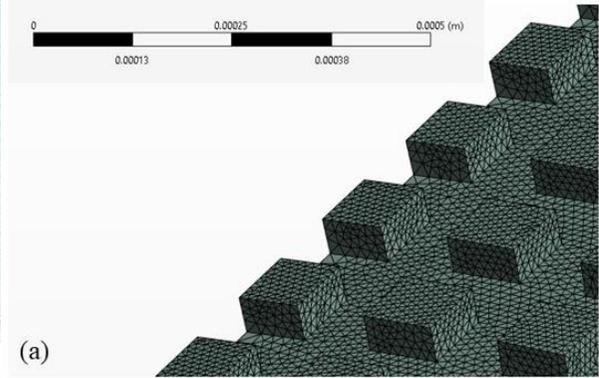
ANALYSIS II: Study of different regular metasurface patterns

Fluid dynamics in baseline simulation without metasurface



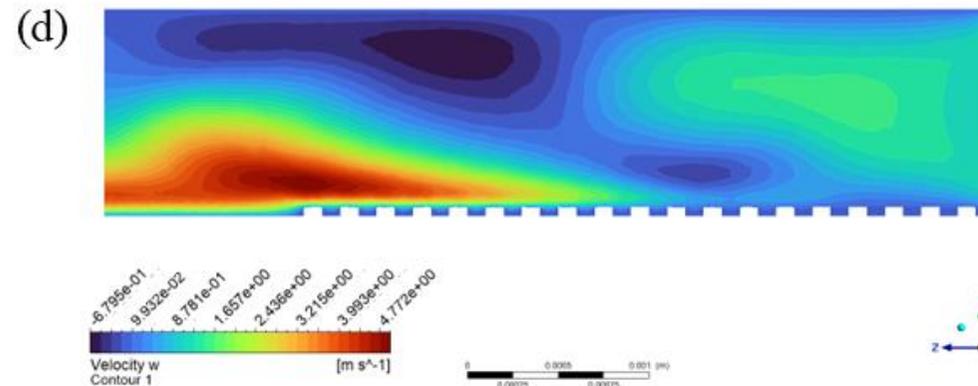
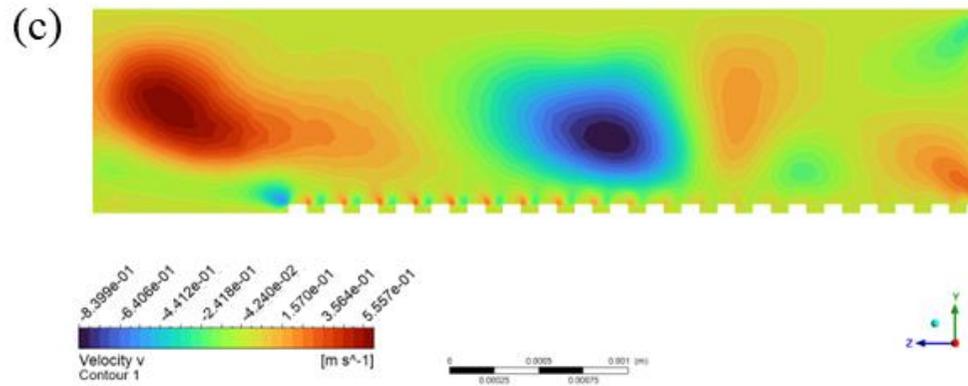
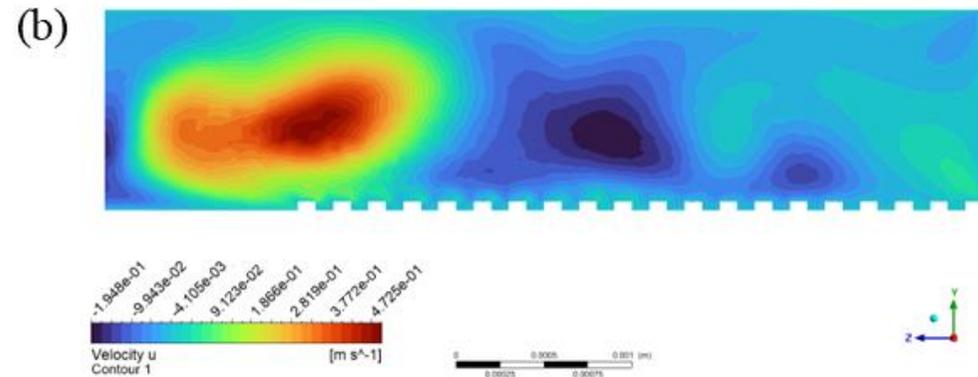
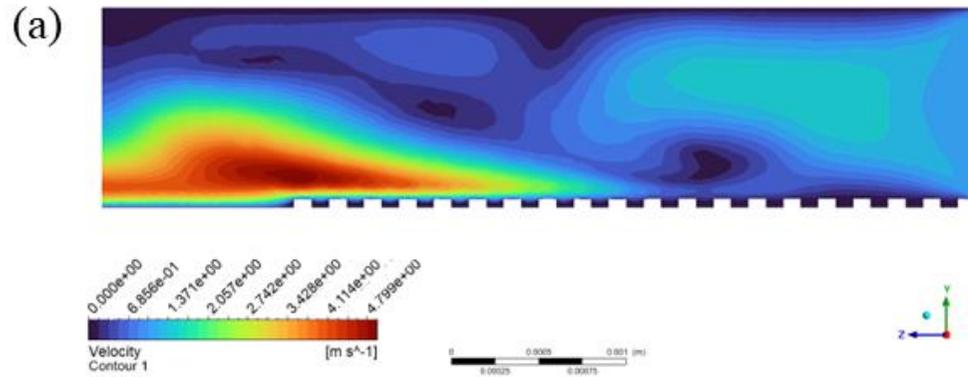
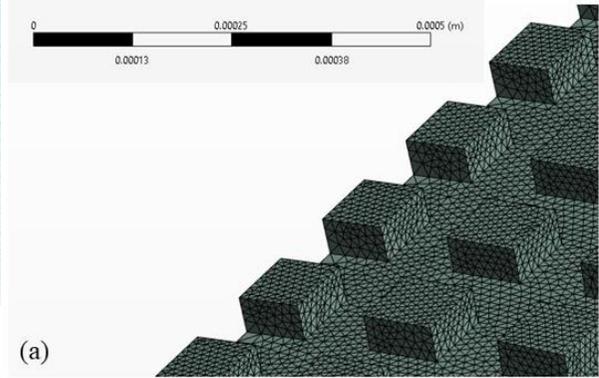
ANALYSIS II: Study of different regular metasurface patterns

Fluid dynamics in the case of small squares (Design #0)



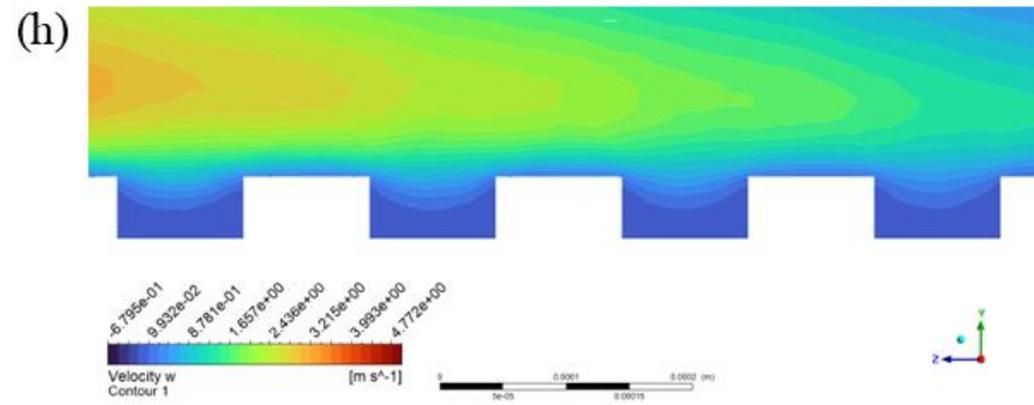
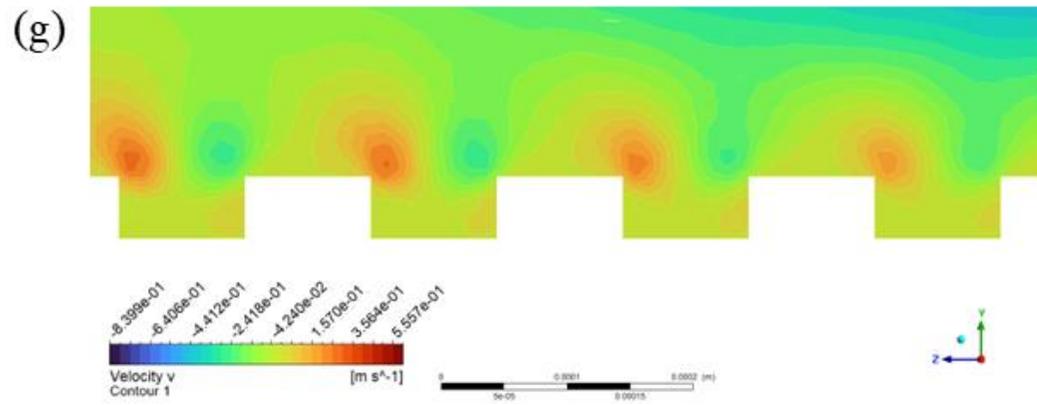
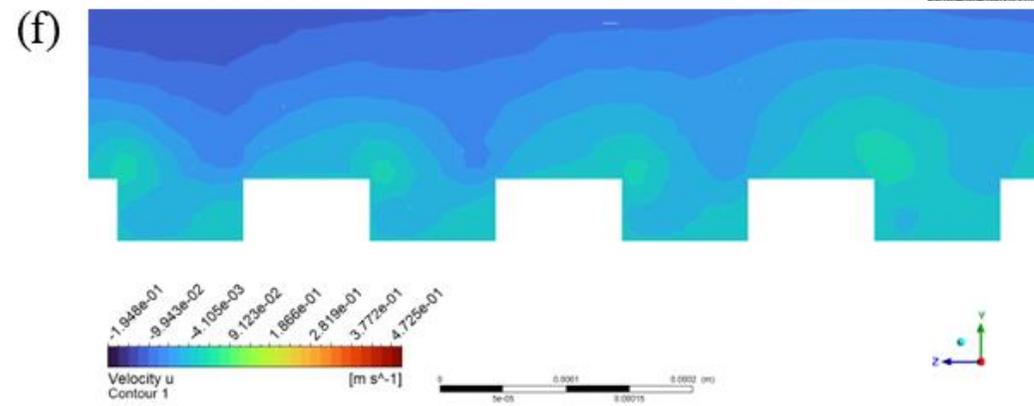
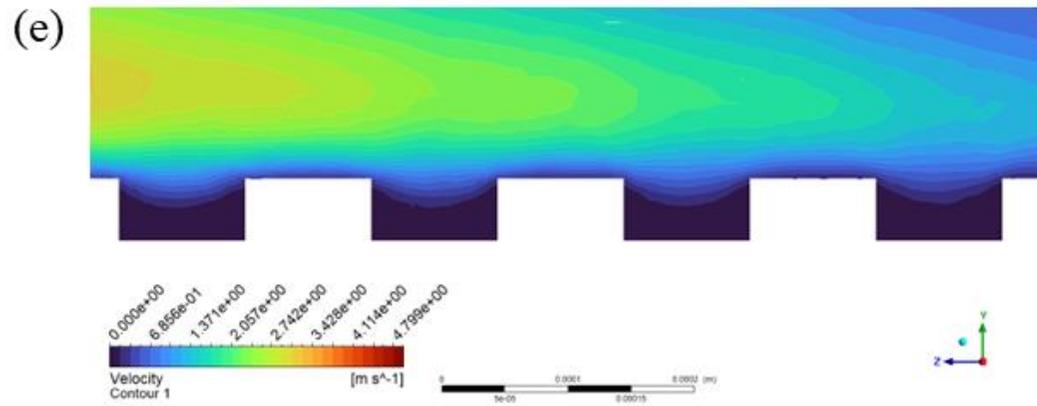
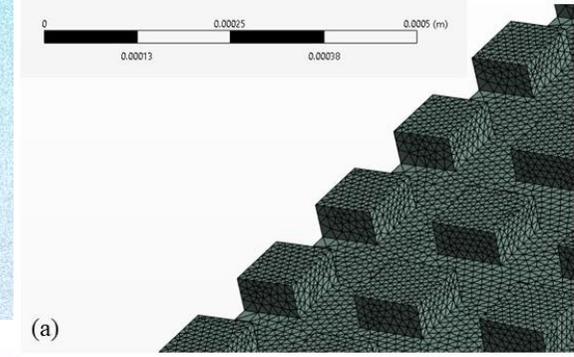
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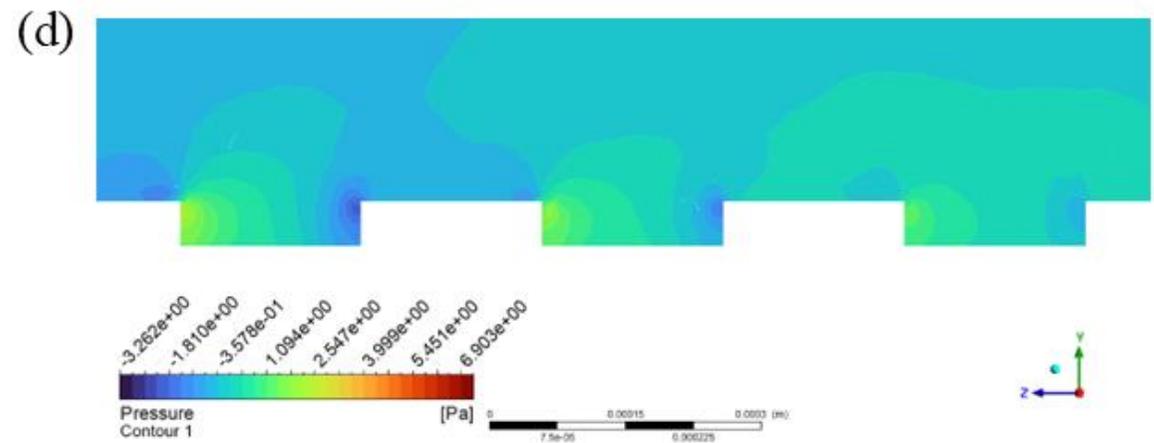
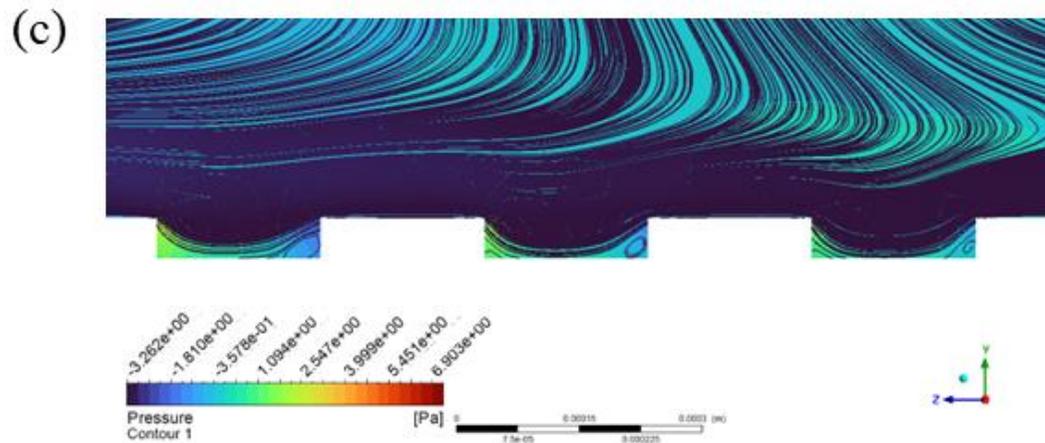
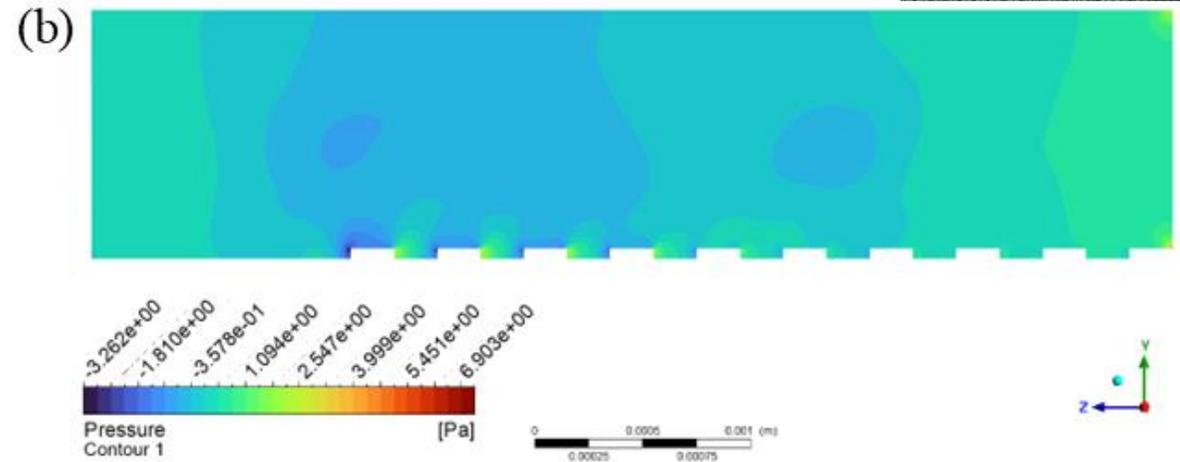
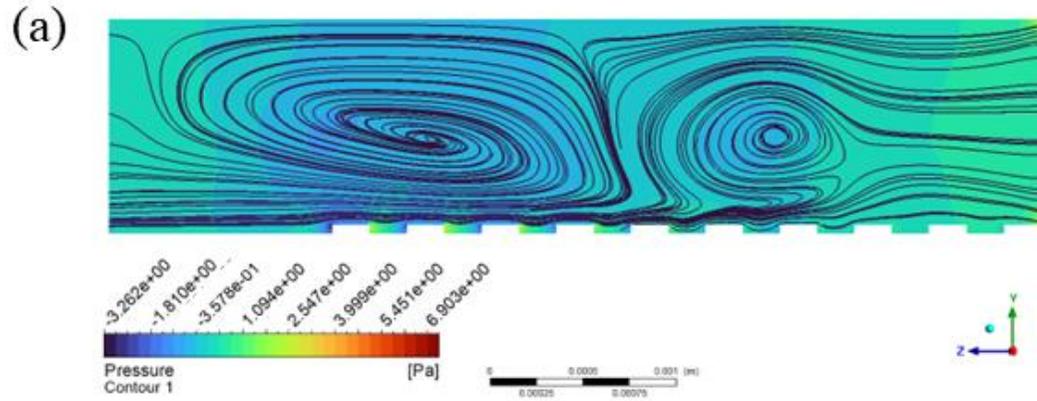
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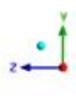
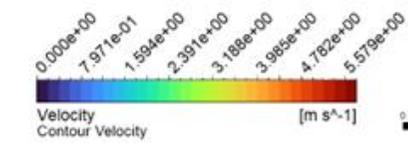
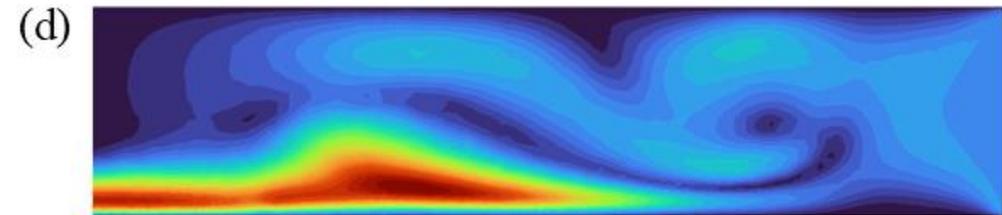
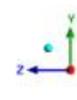
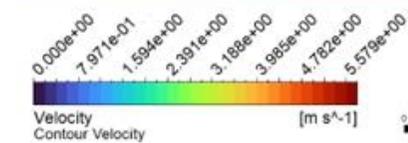
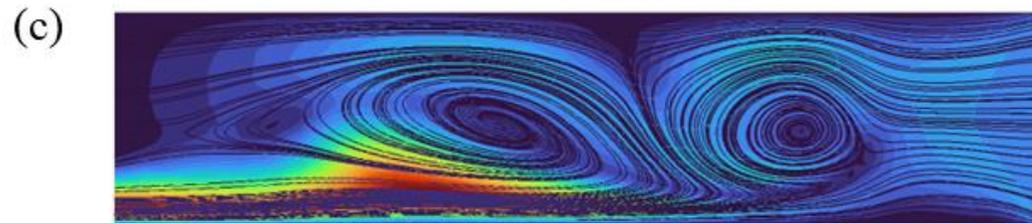
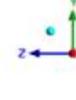
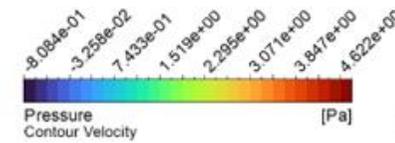
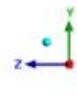
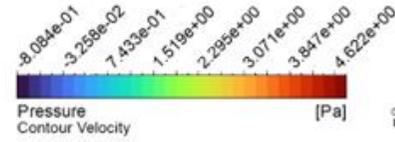
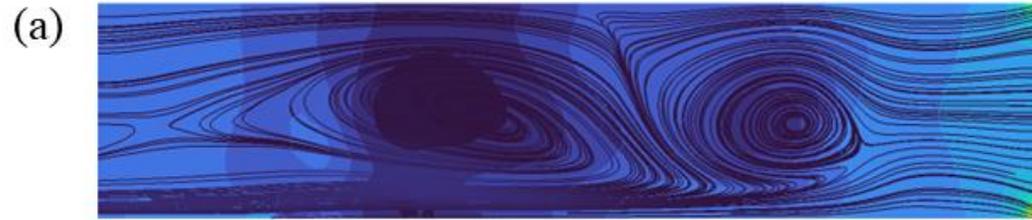
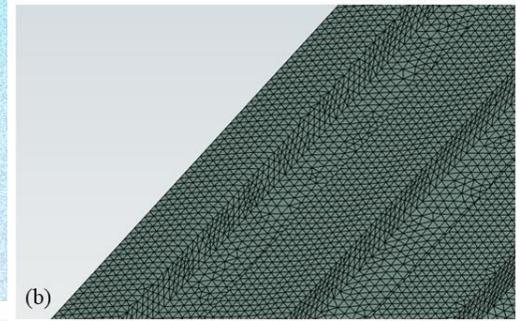
ANALYSIS II: Study of different regular metasurface patterns

Fluid dynamics in the case of large squares



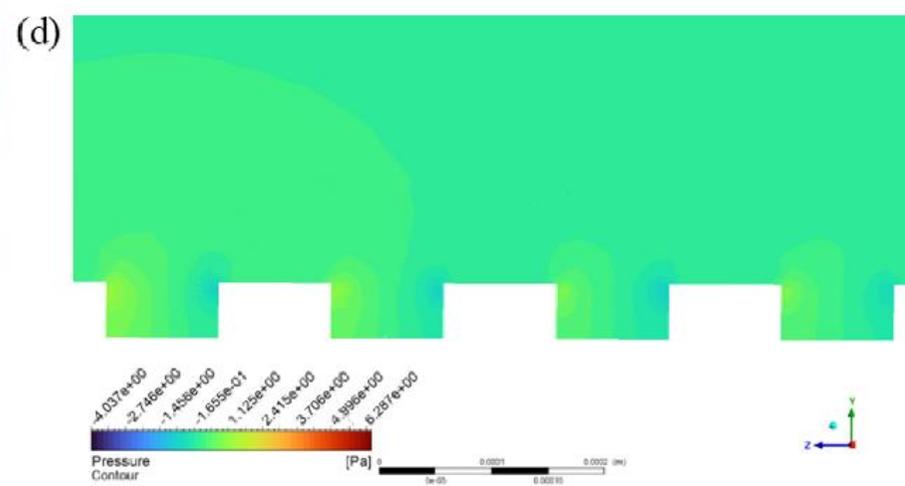
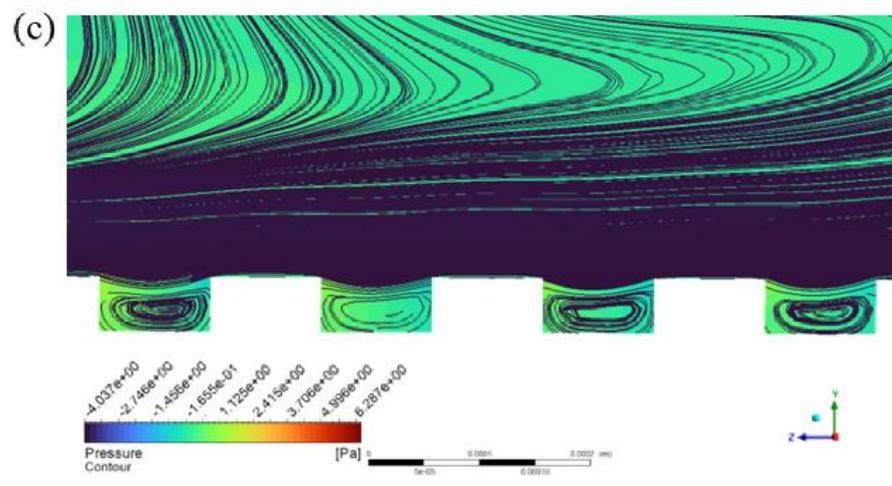
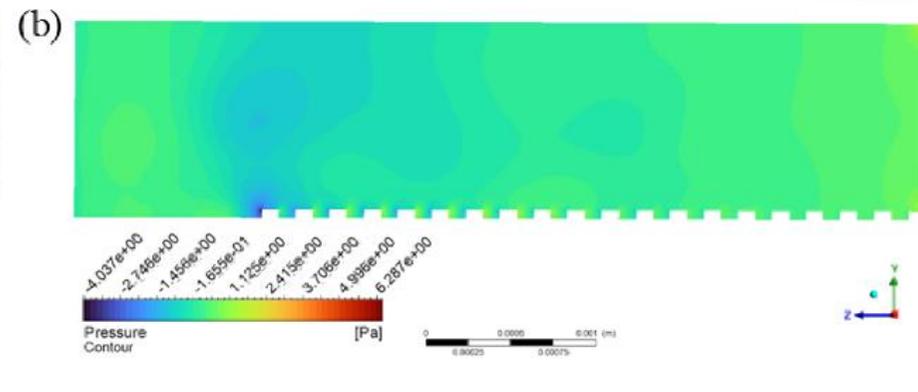
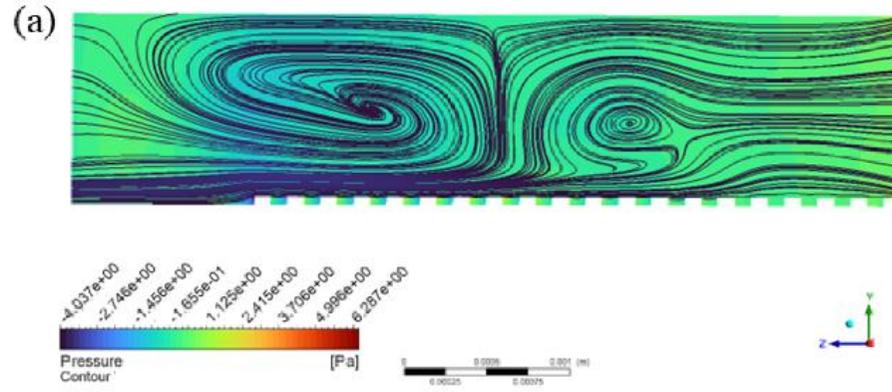
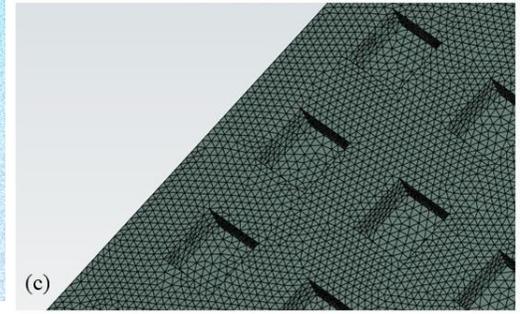
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Fluid dynamics in the case of line-elements



ANALYSIS II: Study of different regular metasurface patterns

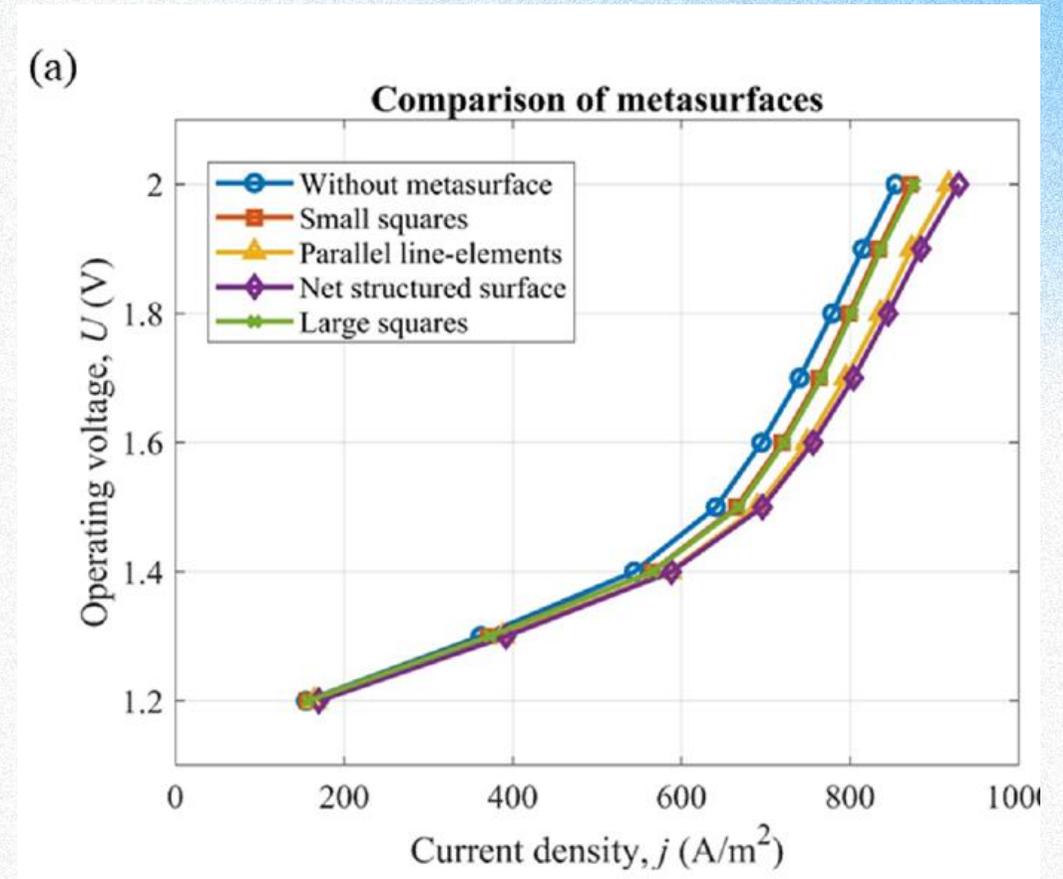
Fluid dynamics in the case of net-structured surface



ANALYSIS II: Study of different regular metasurface patterns

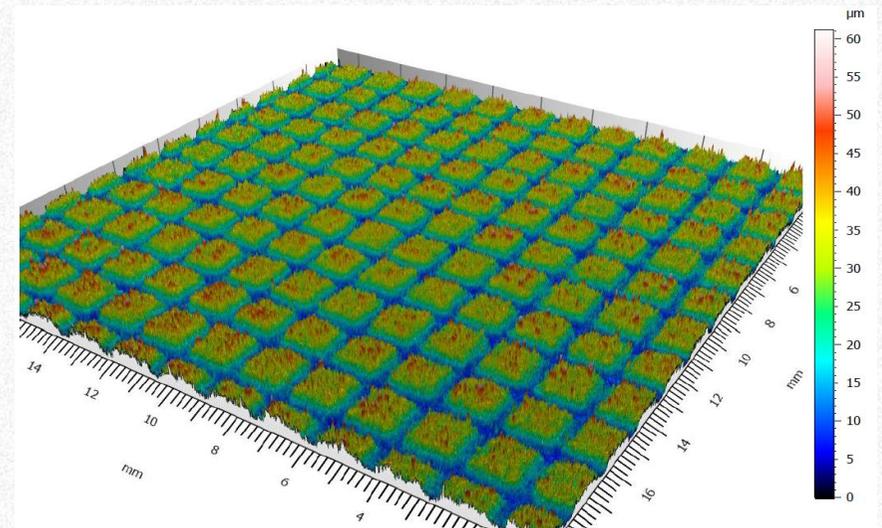
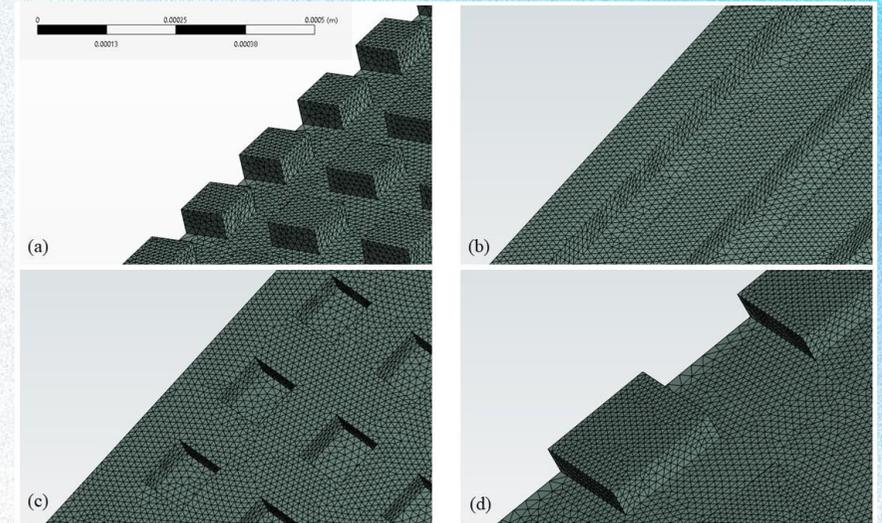
Conclusions from Analysis II:

- ❑ Net-structured metasurface provides increase in the current density characteristics by **8.5%** at the applied voltage 1.5V and could be considered **the most efficient**.
- ❑ Even the optimized rectangular shaped metasurface from Analysis I is less efficient than the not optimized net-structured metasurface.
- ❑ Metasurface leads to additional circulation in the air channel, improving the current density characteristics.
- ❑ Use of metamaterials for solid oxide electrolyzers opens a space of opportunities for improving the device performance by the geometry optimisation.



LIMITATIONS OF THE CURRENT STUDY / DISCUSSION

- ❑ The studied SOEC **was not** optimized in terms of the:
 - operating conditions
 - material composition
 - thickness of layers
 - porosity level
 - other cell characteristics
- ❑ Comparison with Jang and Kelsall (2022), Jang et al. (2022) reveals that anode metasurface is overall **less efficient**, than the metasurface pattern of conical and cylindrical pillars applied to all functional layers of the cell.
- ❑ Fabrication challenge: requires **very precise custom made** meshes.
- ❑ SOEC with metasurface was not studied for short-term and long-term **degradation** scenarios.



Thank you!

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More information in the publication:

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