Norway grants

The National Centre for Research and Development

Warsaw University of Technology

Work Package 2

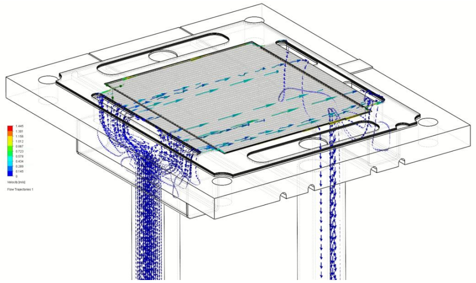
Development and utilization of advanced numerical tools for CCS installations based on MCFC

MOLCAR

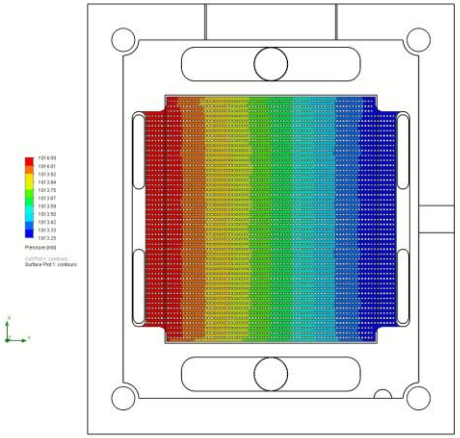
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Work Package 2 (11.2020 .. 10.2022)

Goal: Creating an accurate numerical model of the installation with an MCFC stack for conducting variant analyzes



- Task 2.1: Parametric model
- Task 2.2: Guidelines for the prototype container based installation design
- Task 2.3: Computational fluid mechanics (CFD) model
- Task 2.4: Tuning and validation of a parametric model of the installation from the MCFC
- Task 2.5: Verification of assumptions and optimization of operating parameters

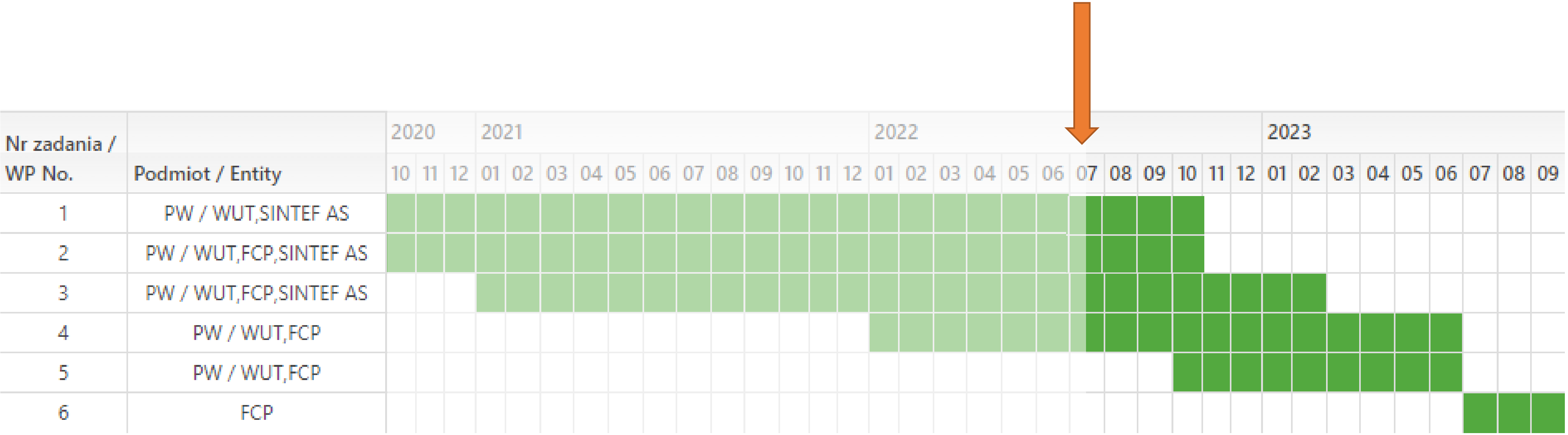


„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Norway grants

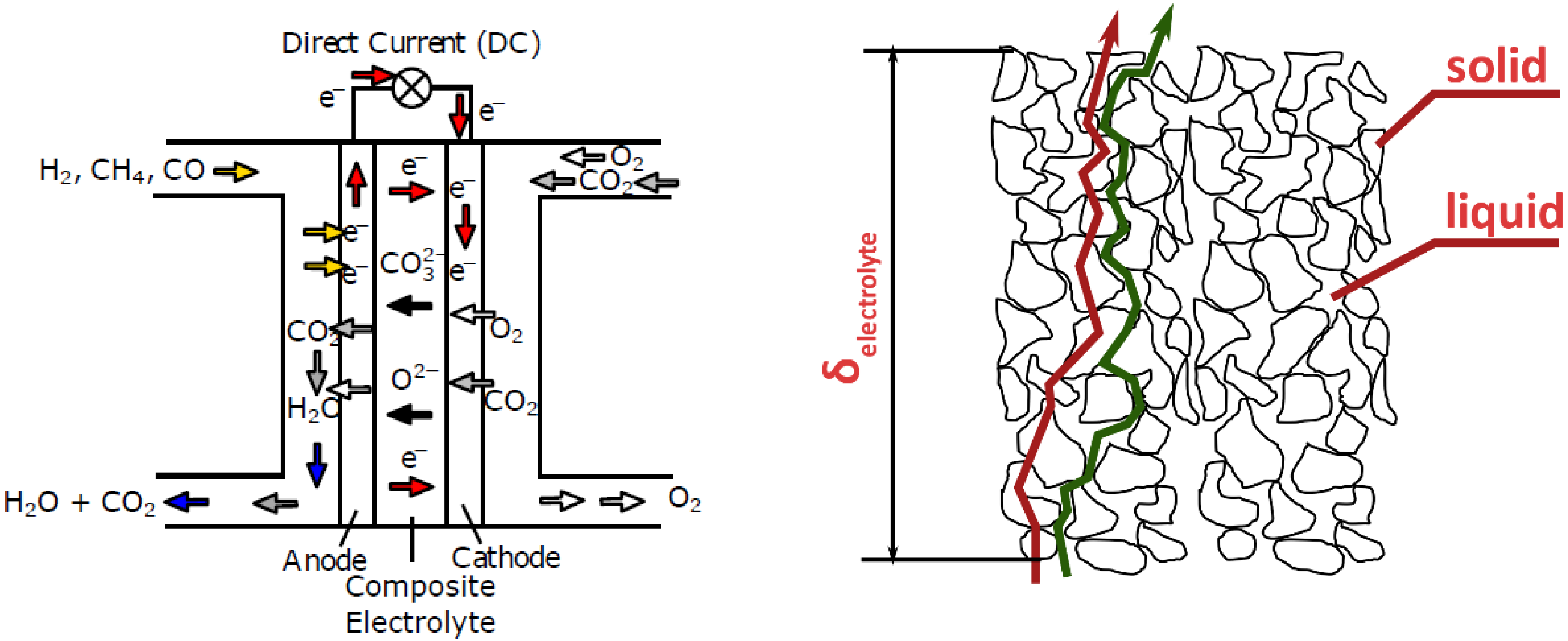
The National Centre for Research and Development

Warsaw University of Technology



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.1: Parametric model



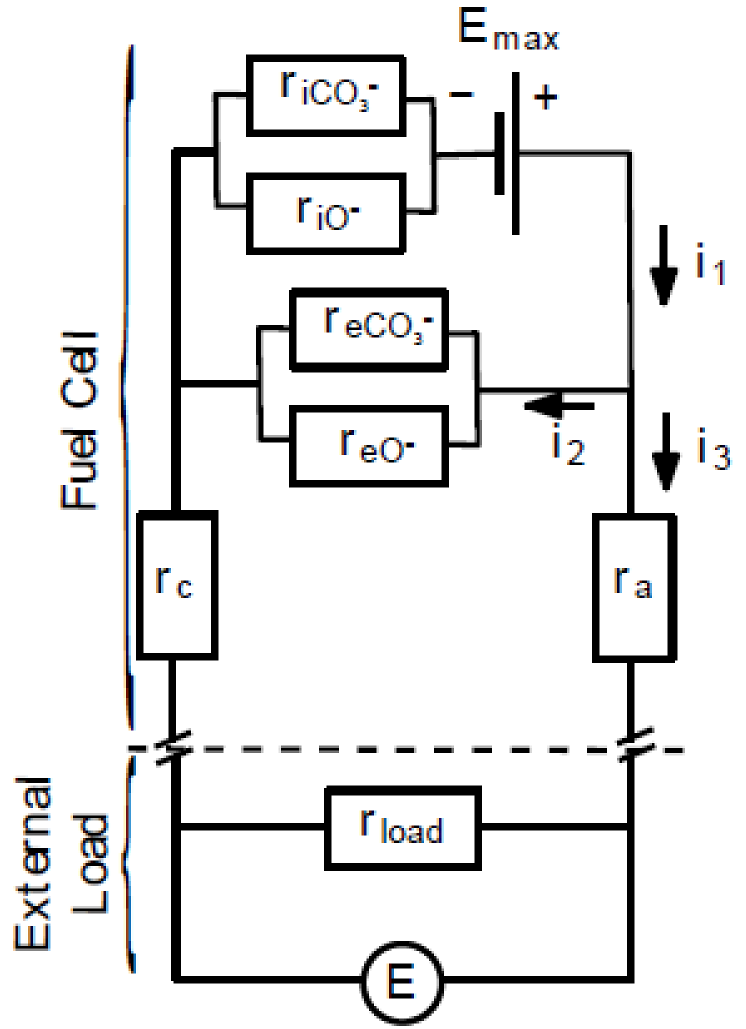
Working principles of a dual conductivity Molten Carbonate Fuel Cell

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.1: Parametric model

$$
\begin{cases}
E_{max} = \dfrac{(i_{iCO_3^=} + i_{iO^=}) \cdot r_{iCO_3^=} \cdot r_{iO^=}}{r_{iCO_3^=} + r_{iO^=}} + \dfrac{(i_{eCO_3^=} + i_{eO^=}) \cdot r_{eCO_3^=} \cdot r_{eO^=}}{r_{eCO_3^=} + r_{eO^=}} \\
E + (r_a + r_c) \cdot i_{load} = \dfrac{(i_{eCO_3^=} + i_{eO^=}) \cdot r_{eCO_3^=} \cdot r_{eO^=}}{r_{eCO_3^=} + r_{eO^=}} \\
i_{load+}i_{eCO_3^=} + i_{eO^=} = i_{iCO_3^=} + i_{iO^=} \\
r_{iCO_3^=} \cdot i_{iO^{==}} = r_{iO^=} i_{iO^=} \\
r_{eCO_3^=} \cdot i_{eO^=} = r_{eO^=} \cdot i_{eO^=}
\end{cases}
$$

$$
E = \frac{E_{max} - i_{load} \dfrac{r_{iO^=} \cdot r_{iCO_3^=}}{r_{iO^=} + r_{iCO_3^=}} (r_a + r_c)\left(1 + \dfrac{1}{r_{iCO_3^=}} + \dfrac{1}{r_{iO^=}} + \dfrac{1}{r_{eO^=}} + \dfrac{1}{r_{eCO_3^=}}\right)}{1 + \dfrac{r_{iO^=}}{r_{iO^=} + r_{iCO_3^=}} \dfrac{r_{iCO_3^=}}{r_{eCO_3^=}} + \dfrac{r_{iCO_3^=}}{r_{iO^=} + r_{iCO_3^=}} \dfrac{r_{iO^=}}{r_{eO^=}}}
$$



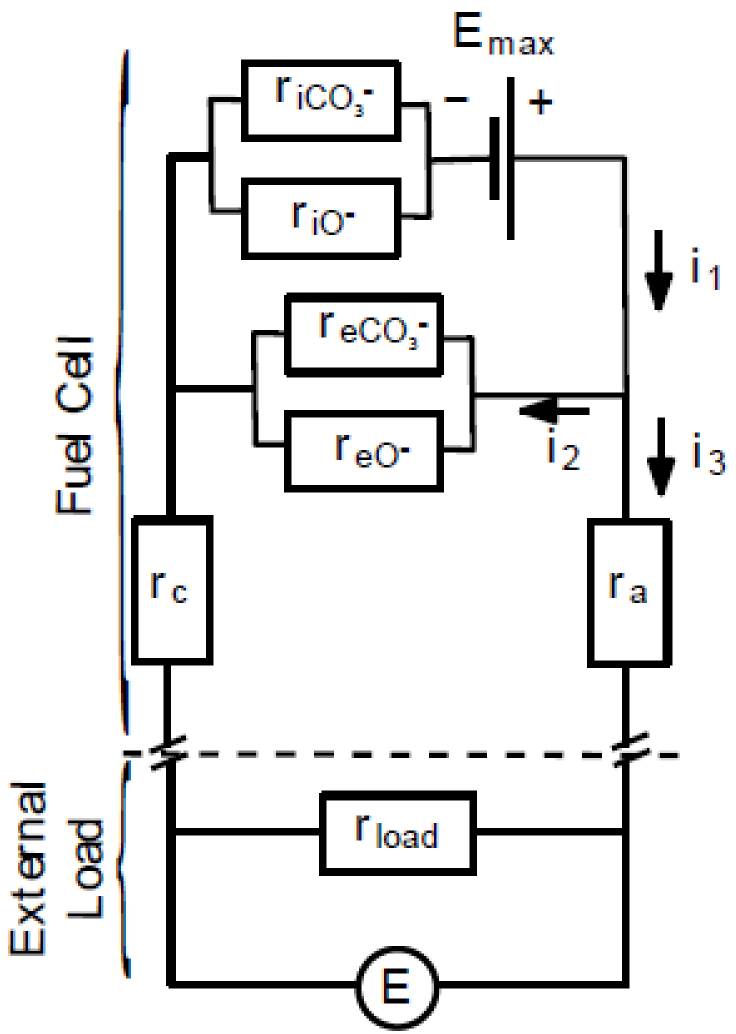
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.1: Parametric model

$$r = \frac{\delta}{\sigma_{CO_3^{=}} \cdot \rho + \sigma_{O^{=}} \cdot (1 - \delta)}$$

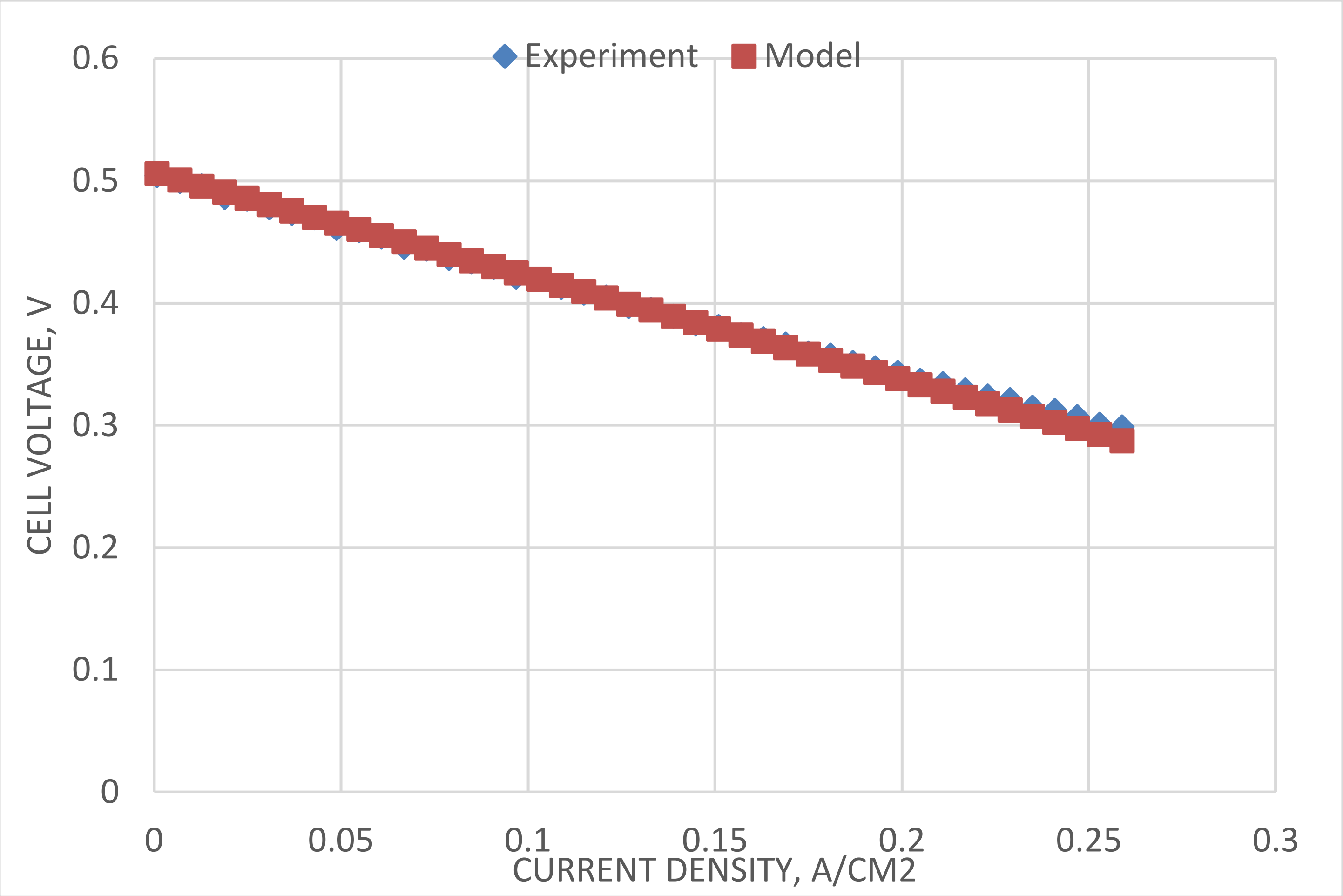
$$\sigma = \sigma_0 e^{\frac{-E_{act}}{R \cdot T}}$$

	σ_0, S/cm	E_{act}, mol/kJ
Li_2CO_3/K_2CO_3 eutectic [82]	3.59	25.1
SDC	73.5	60.2
BNT (this study)	**1250**	**133**
LNT (this study)	**6020**	**152**
Yttrium Stabilized Zirconia (this study)	**391**	**87.8**



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

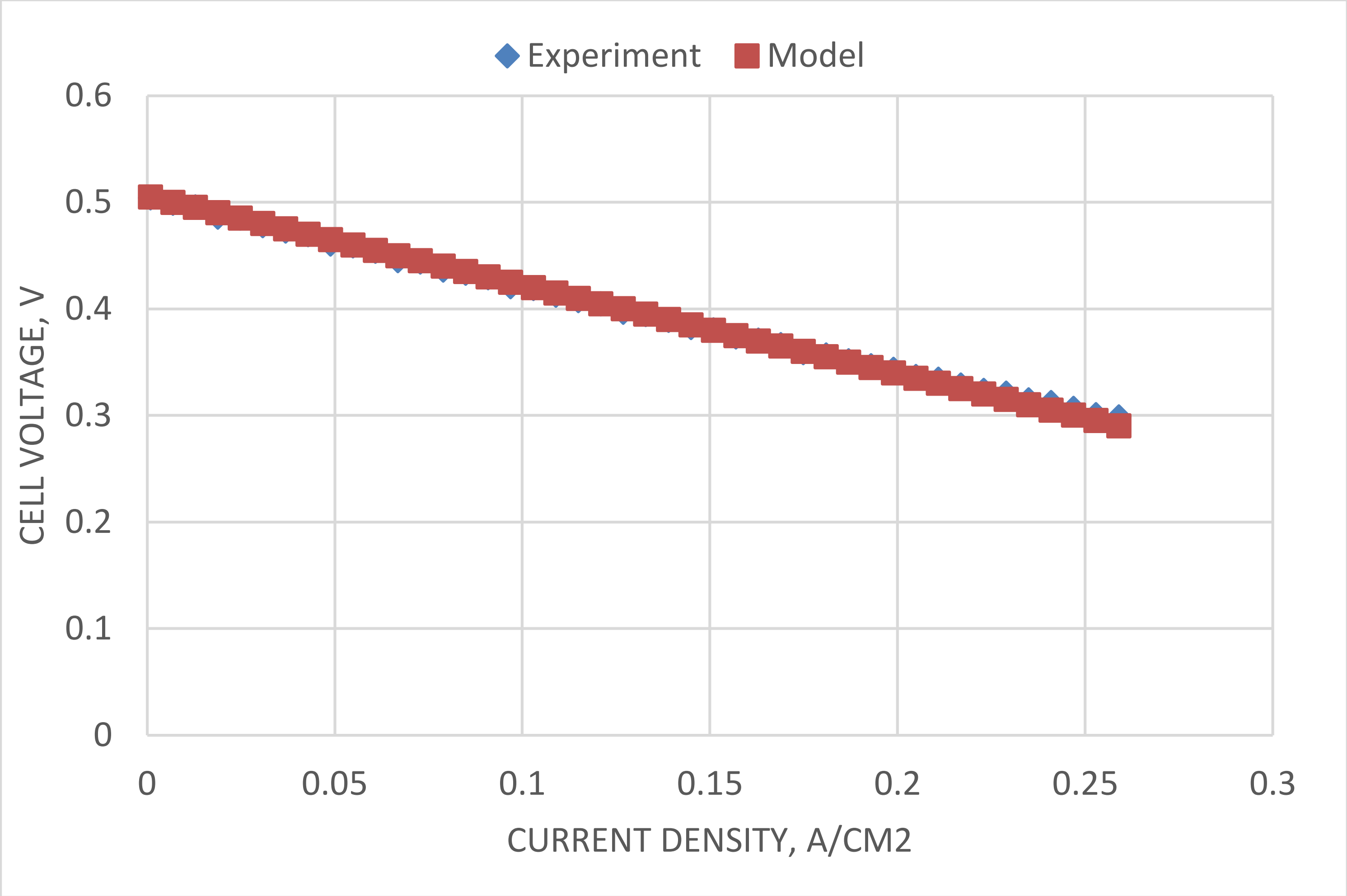
Task 2.1: Parametric model – Li_2CO_3/K_2CO_3-BNT model



Model validation results for double conductivity electrolyte liK-BNT (Cell 1), tortuosity of BNT 25, tortuosity of LiK 6.6; r_eCO3 of LiK 1.64 Ohm x cm2, r_eO of BNT 179 Ohm x cm2

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

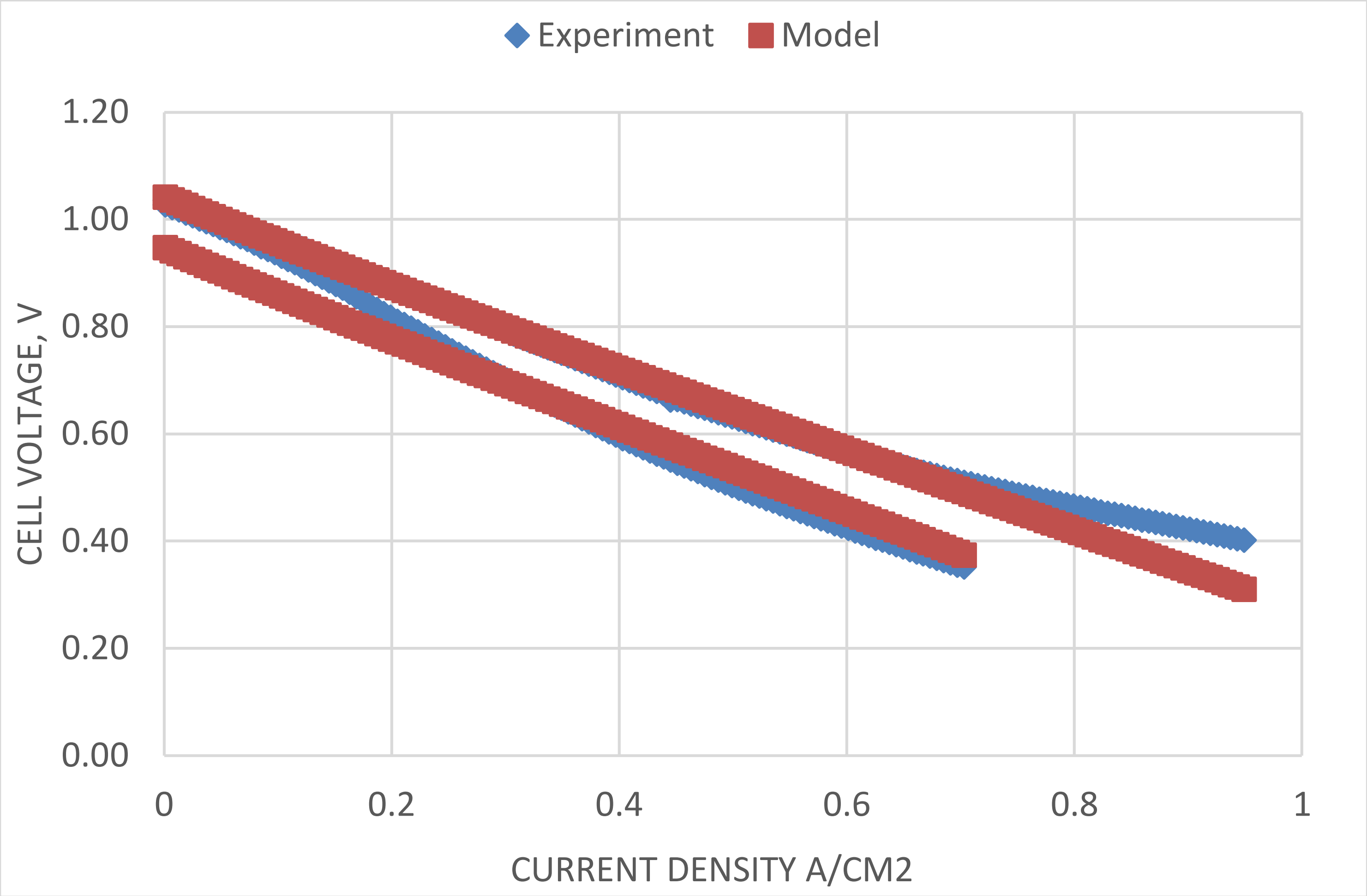
Task 2.1: Parametric model – Li_2CO_3/K_2CO_3-BNT model



Model validation results for double conductivity electrolyte LiK-BNT (Cell 2), tortuosity of BNT 0.0009 tortuosity of LiK 61; r_eCO3 of LiK 1.59 Ohm x cm2, r_eO of BNT 35 Ohm x cm2

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

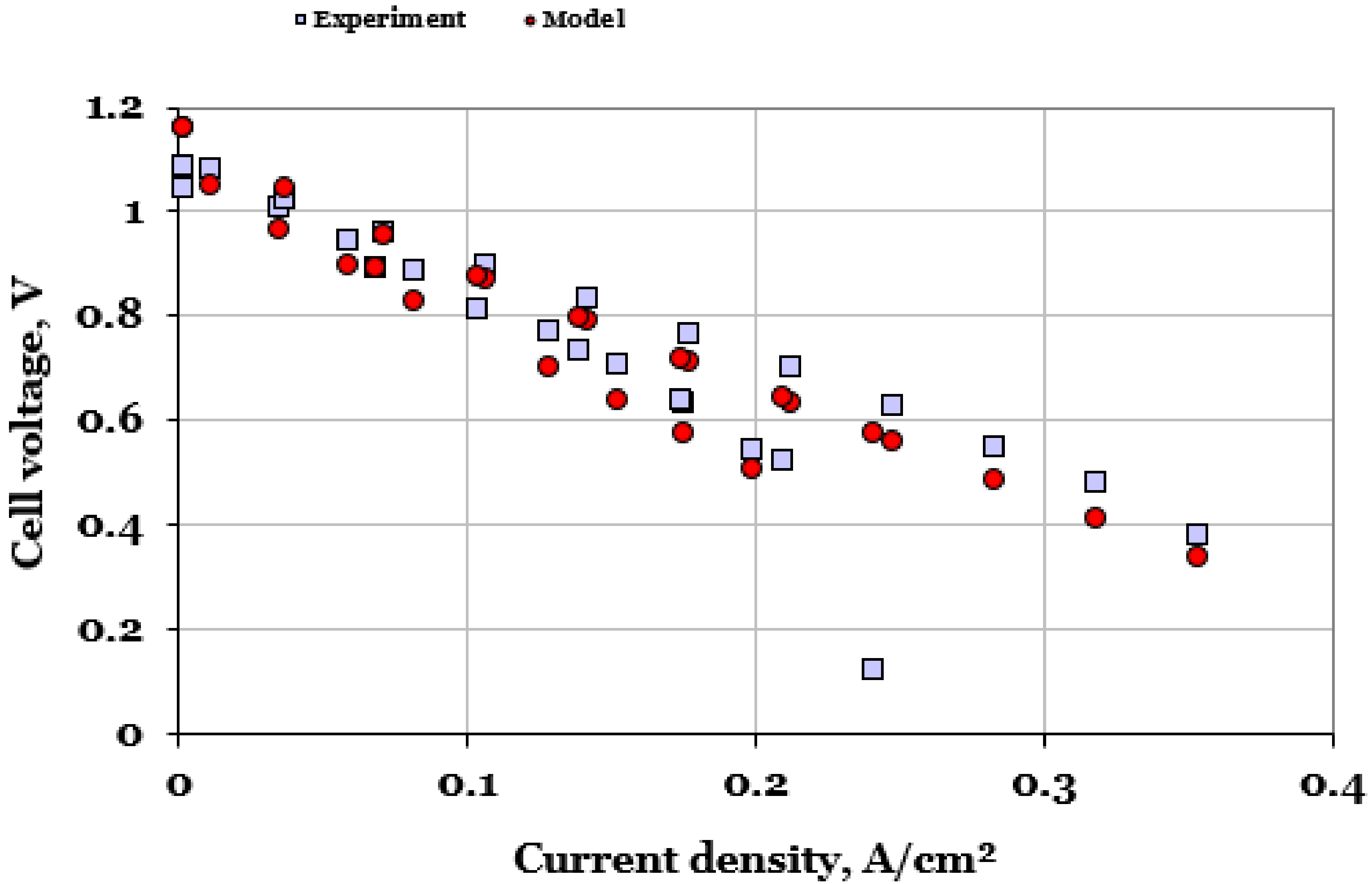
Task 2.1: Parametric model – Li_2CO_3/K_2CO_3-LNT model



Model validation results for double conductivity electrolyte liK-LNT, tortuosity of LNT 0.00064, tortuosity of LiK 7.9; r_eCO3 of LiK 6.2 Ohm x cm^2, r_eO of LNT 1540 Ohm x cm^2

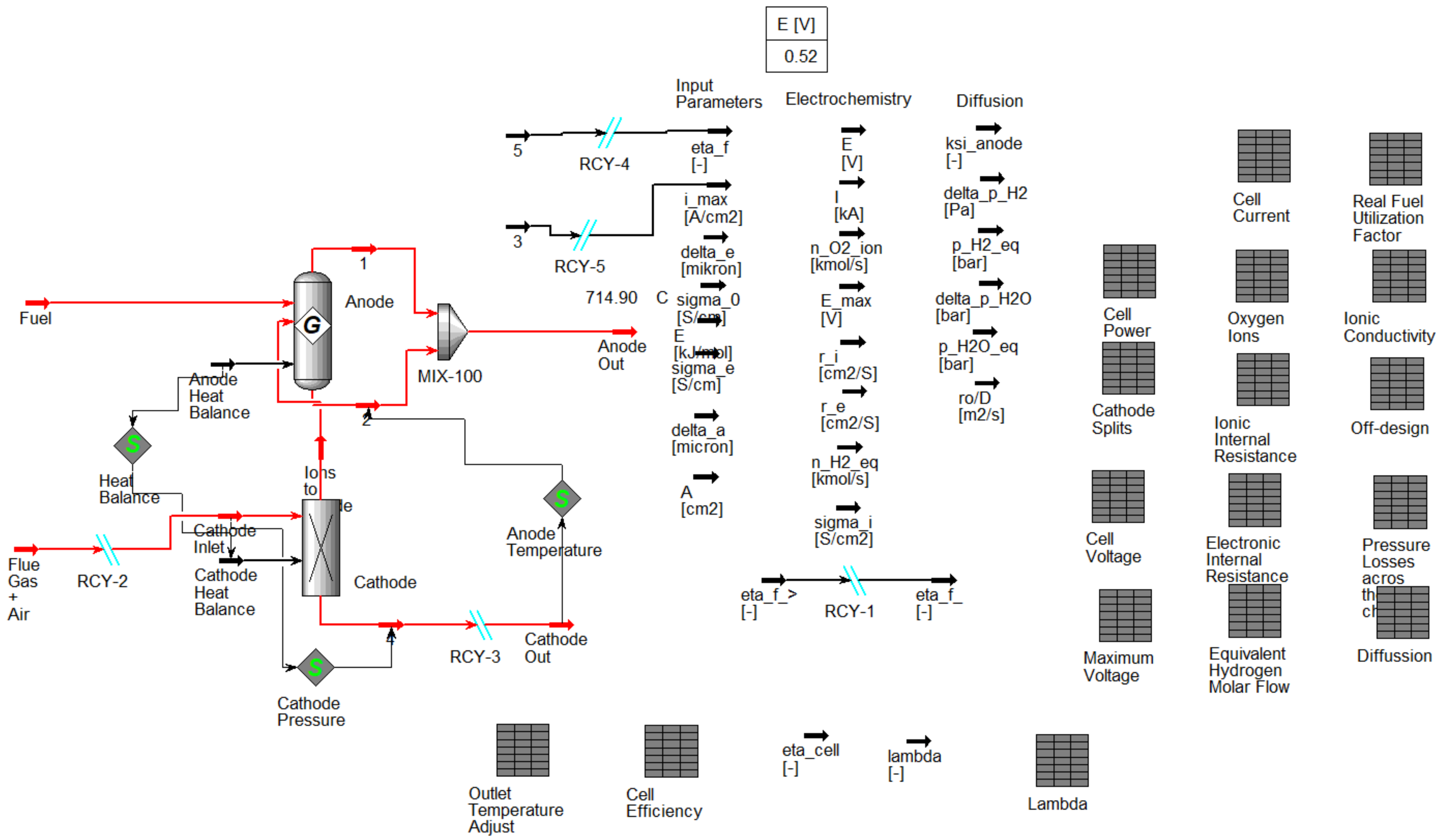
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.1: Parametric model – Li_2CO_3/K_2CO_3-YSZ model



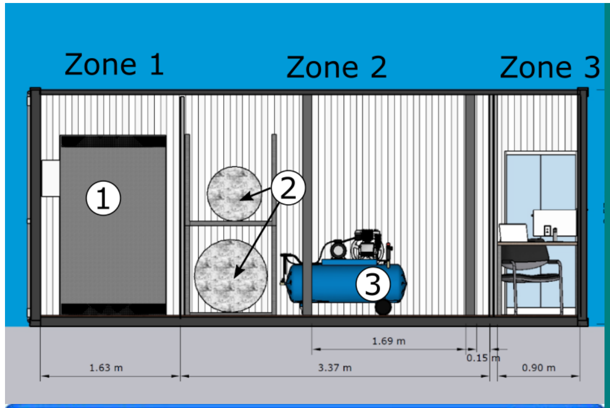
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.1: Parametric model implementation into Aspen HYSYS



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.2: Guidelines for the prototype container based installation design



Cathode split

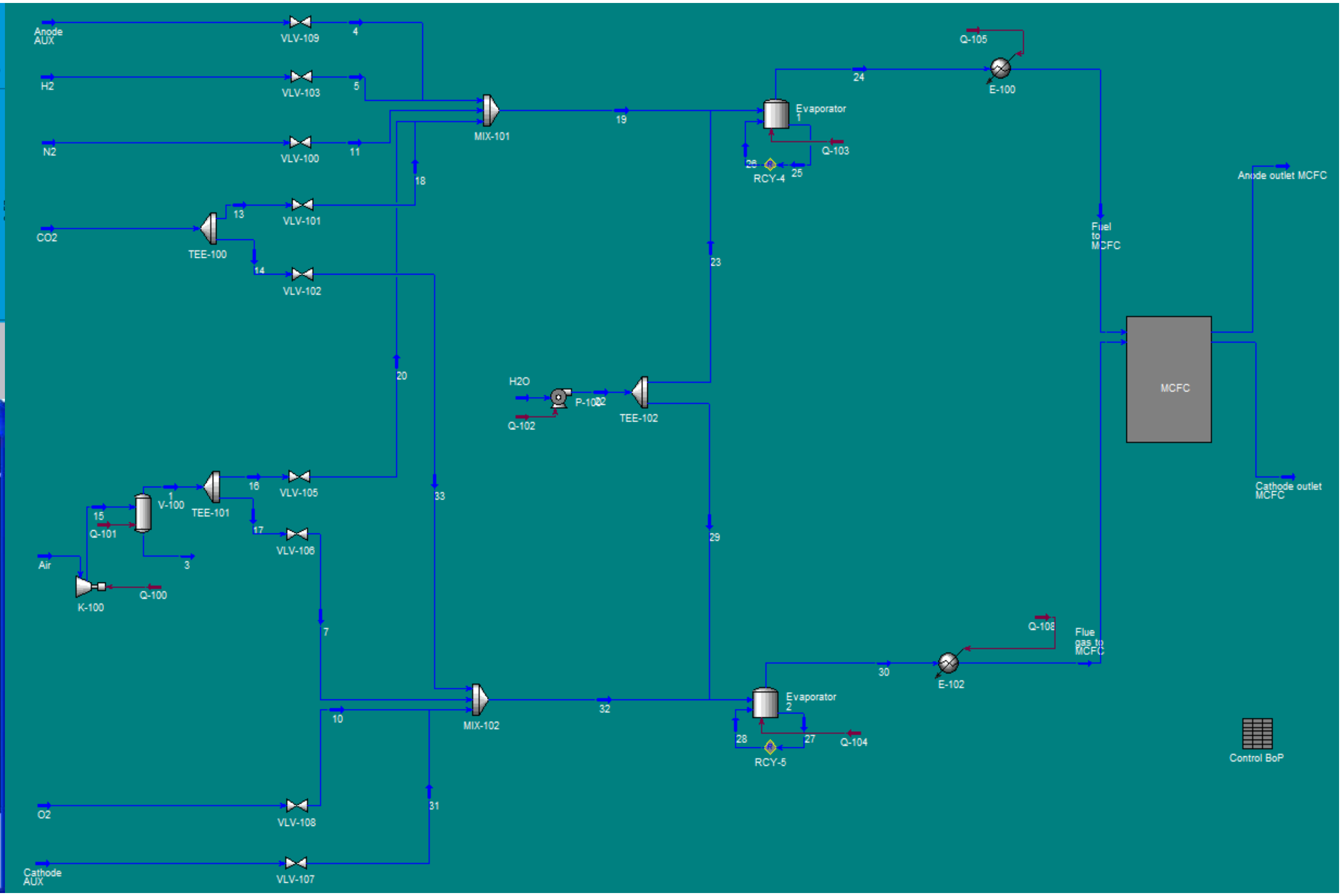
Current Cell

A10 Variable: Exportable Angles in:

	A	B	C
1	oxygen inlet	0.0001 gmole/s	
2	co2 inlet	0.0002 gmole/s	
3	oxygen outlet	1.880e-005	
4	co2 outlet	3.759e-005	
5	oxygen in	0.0001 gmole/s	
6	co2 in	0.0002 gmole/s	
7	oxygen/co2 outlet	0.5000	
8	oxygen out/in	0.1600	
9	co2 out/in	0.2000	
10			

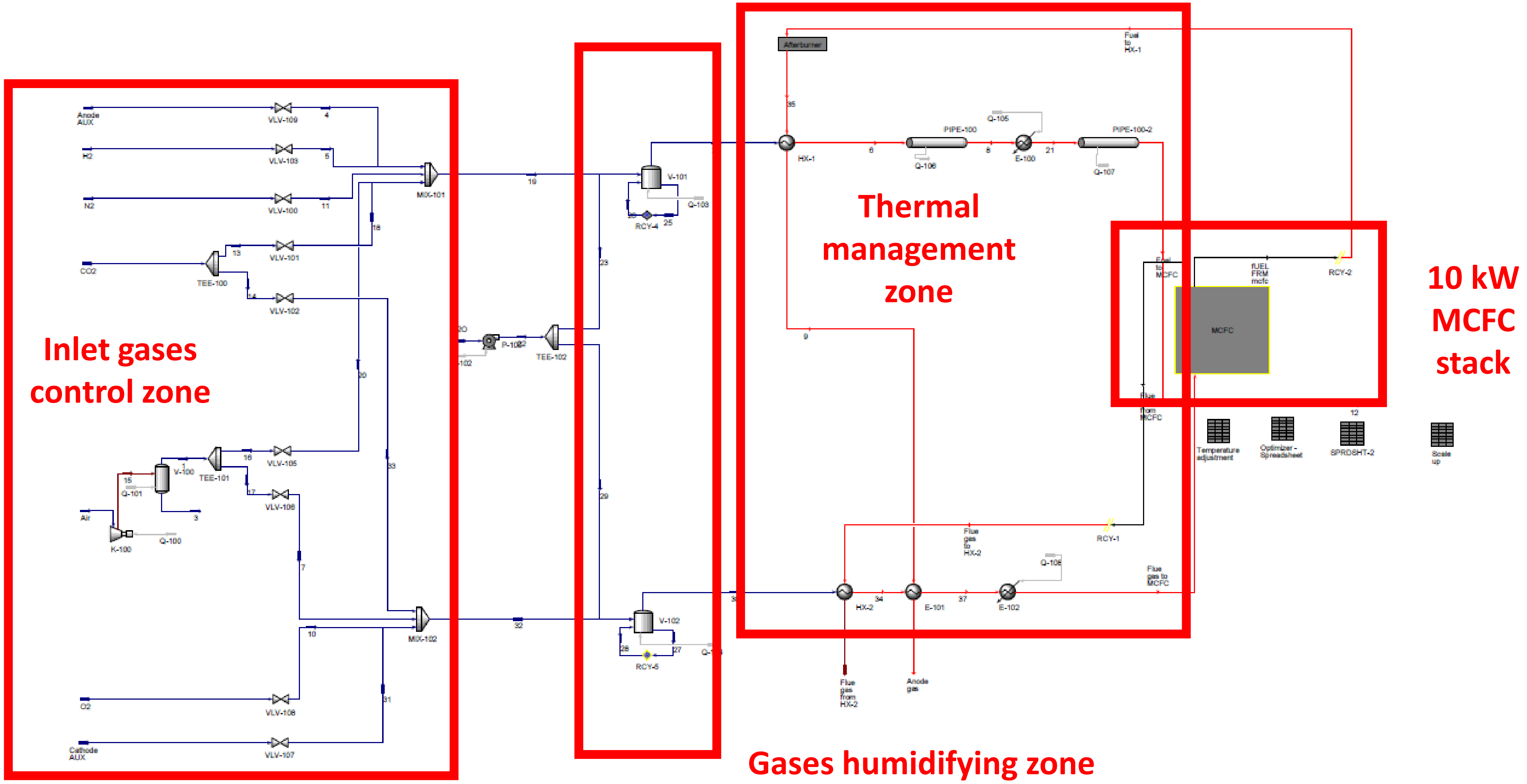
Connections / Parameters / Formulas / Spreadsheet / Calculation Order / ...les

Delete | Function Help... | Spreadsheet Only... | Ignored



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.2: Guidelines for the prototype container based installation design



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.2: Guidelines for the prototype container based installation design

A proposed configuration of flows regulating system, proposed by results of the parametric BoP model.

N	Working medium	Flow rate, NL/min		I/O signal	P-in	P-out
		min	max			
1	Air	5	1800	4..21 mA	2.5	0.5
2	Air	1	300	4..21 mA	2.5	0.5
3	Air	0	33	4..21 mA	2.5	0.5
4	CO2	7.5	300	4..21 mA	2.5	0.5
5	CO2	0.1	15	4..21 mA	2.5	0.5
6	CO2	0	35	4..21 mA	2.5	0.5
7	N2	5	300	4..21 mA	2.5	0.5
8	N2	12	500	4..21 mA	2.5	0.5
9	H2	0	5	4..21 mA	2.5	0.5
10	H2	6	250	4..21 mA	2.5	0.5

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.2: Guidelines for the prototype container based installation design

A proposed configuration of heating system, proposed by results of the parametric BoP model

N	Working medium	Power rate, kW		T_max, C deg
		min	max	
1	Cathodic main electric heater	10	15	800
2	Cathodic supporting electric heater	1.2	3	900
3	Anodic main electric heater	2	5	800
4	Anodic supporting electric heater	1.2	3	900
5	Water steam generator	1.3	3	400

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

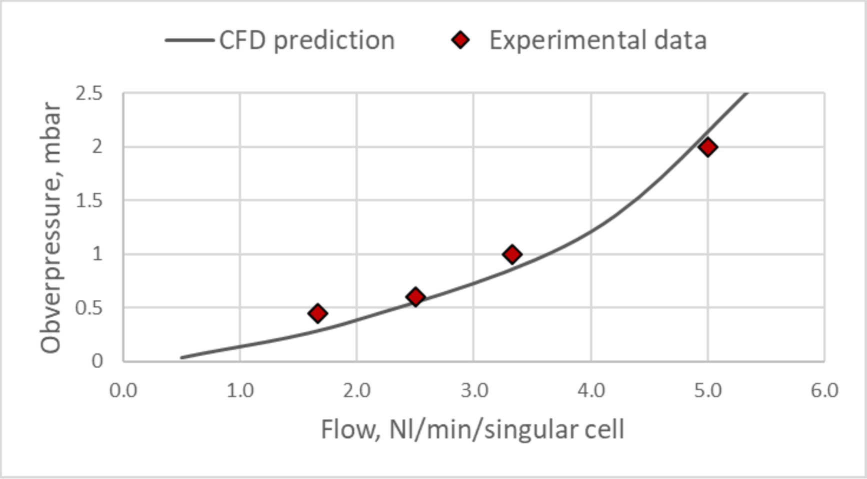
Task 2.2: Guidelines for the prototype container based installation design

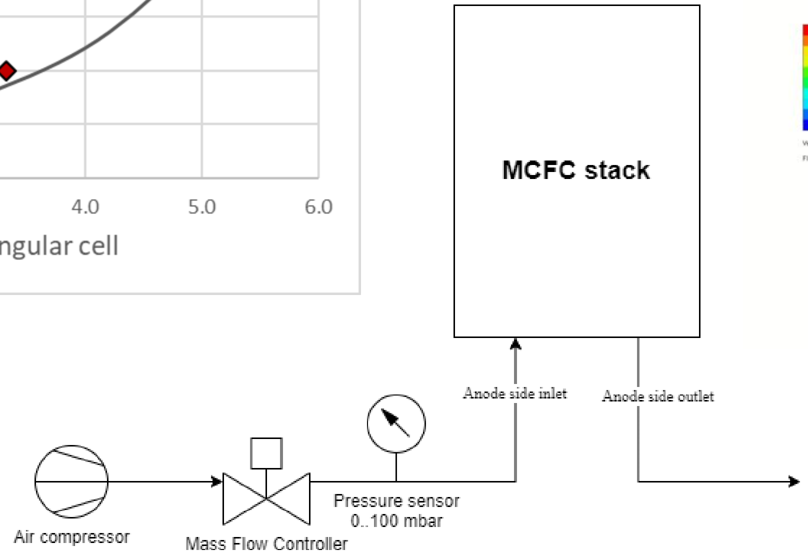
A proposed configuration of electronic load system, proposed by results of the parametric BoP model

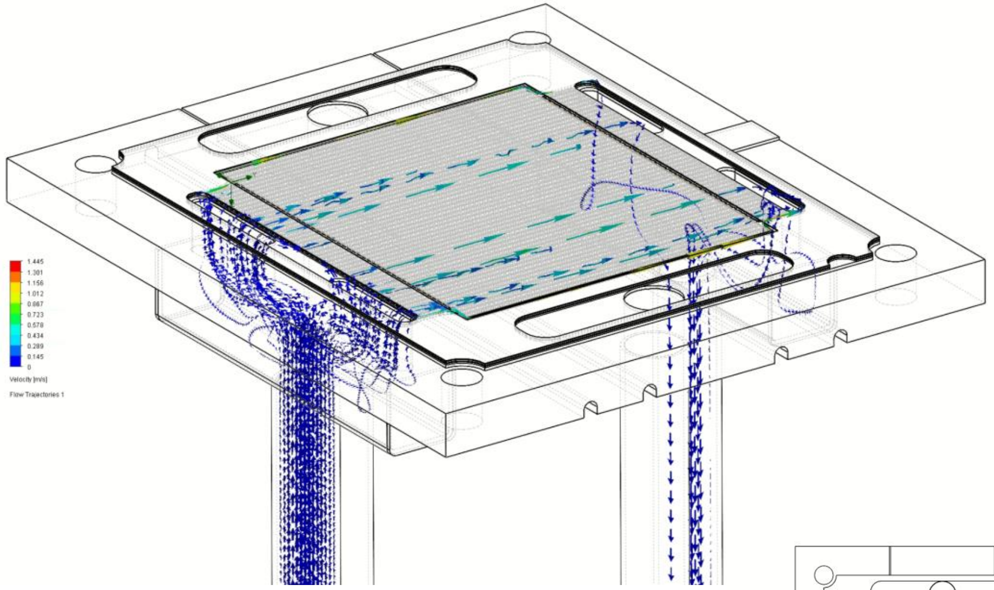
N	Device type	Operating voltage, V		Operating current, A		Sircuit
		min	max	min	max	
1	Electronic load	5	300	0	150	DC

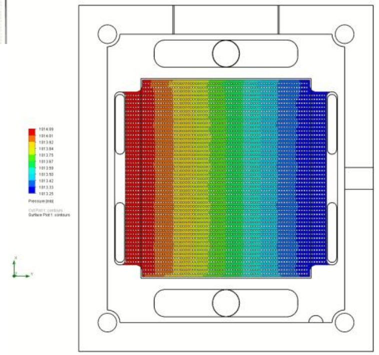
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.3: Computational fluid mechanics (CFD) model



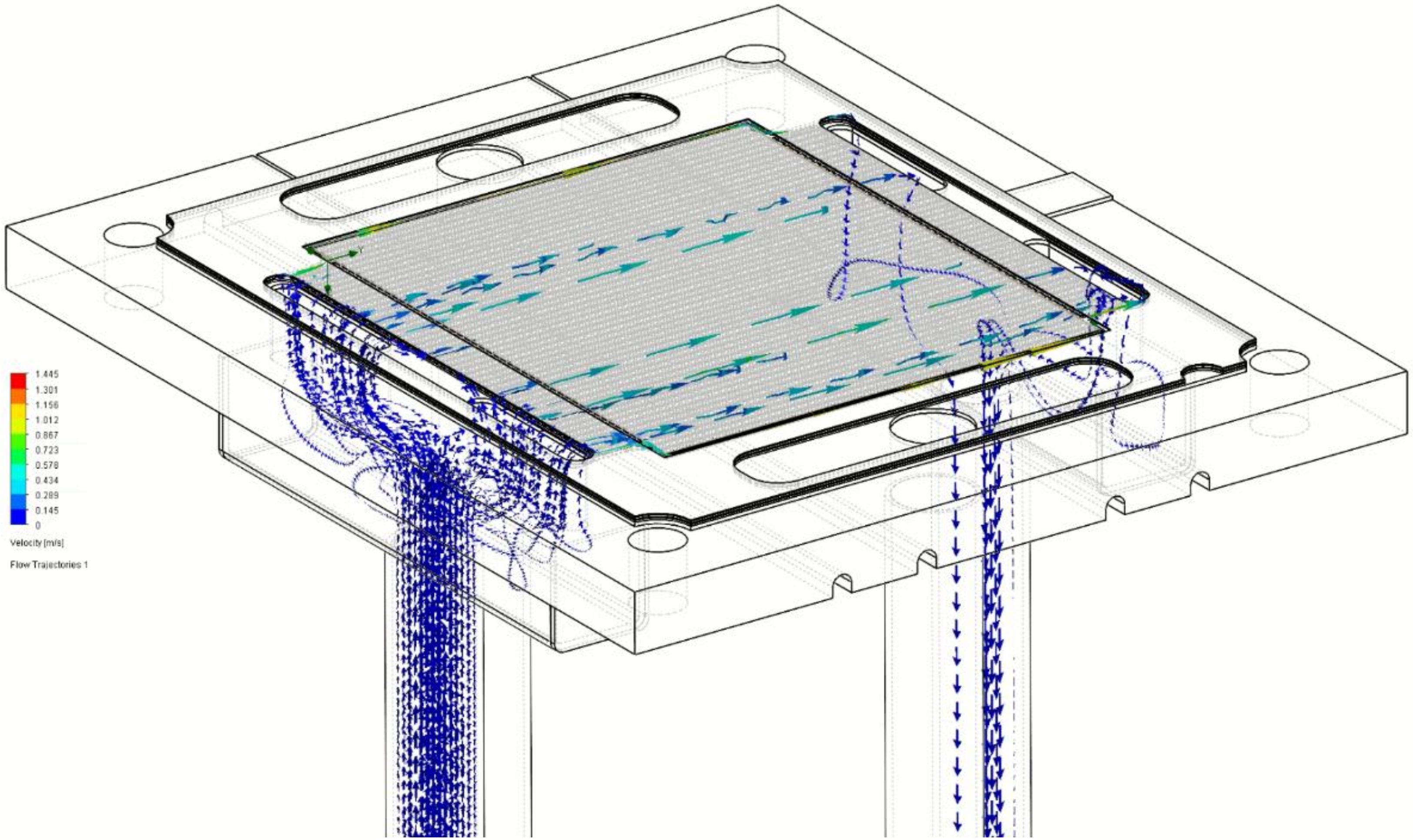






„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

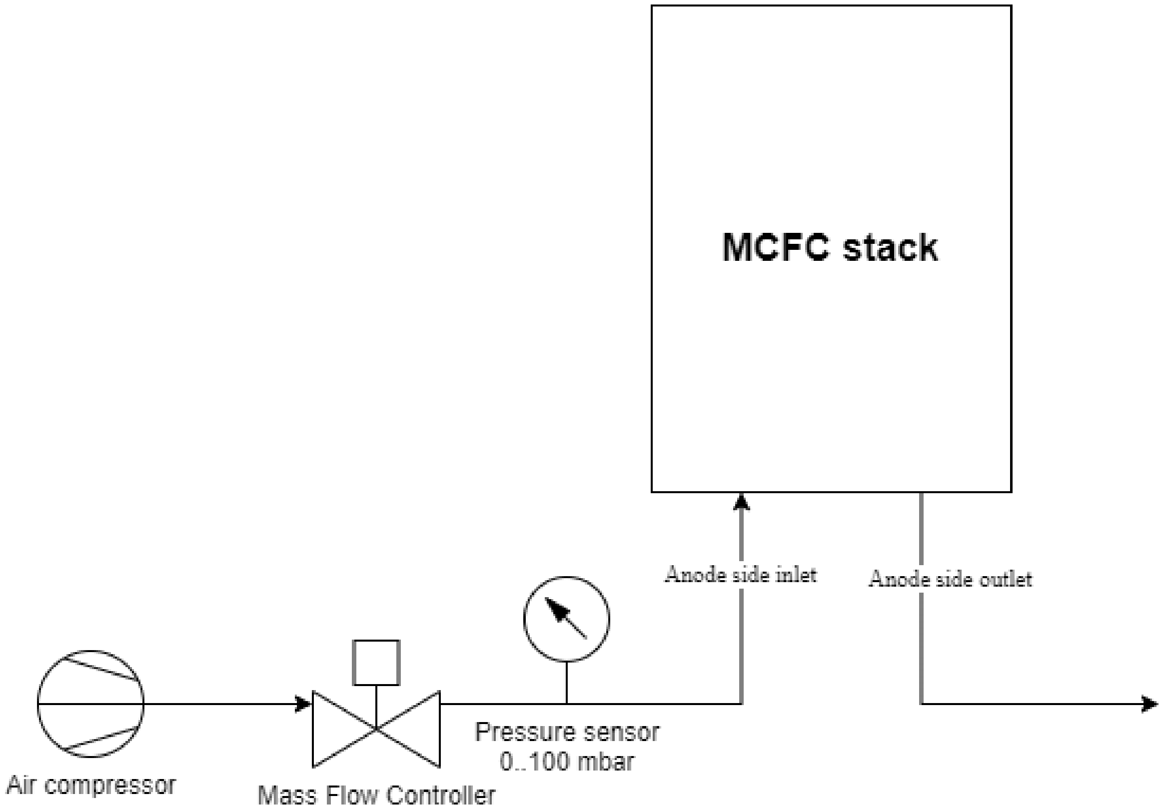
Task 2.3: Computational fluid mechanics (CFD) model



- Internal flow distribution study and optimization
- Anodic and cathodic channels geometry estimation

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.3: Computational fluid mechanics (CFD) model

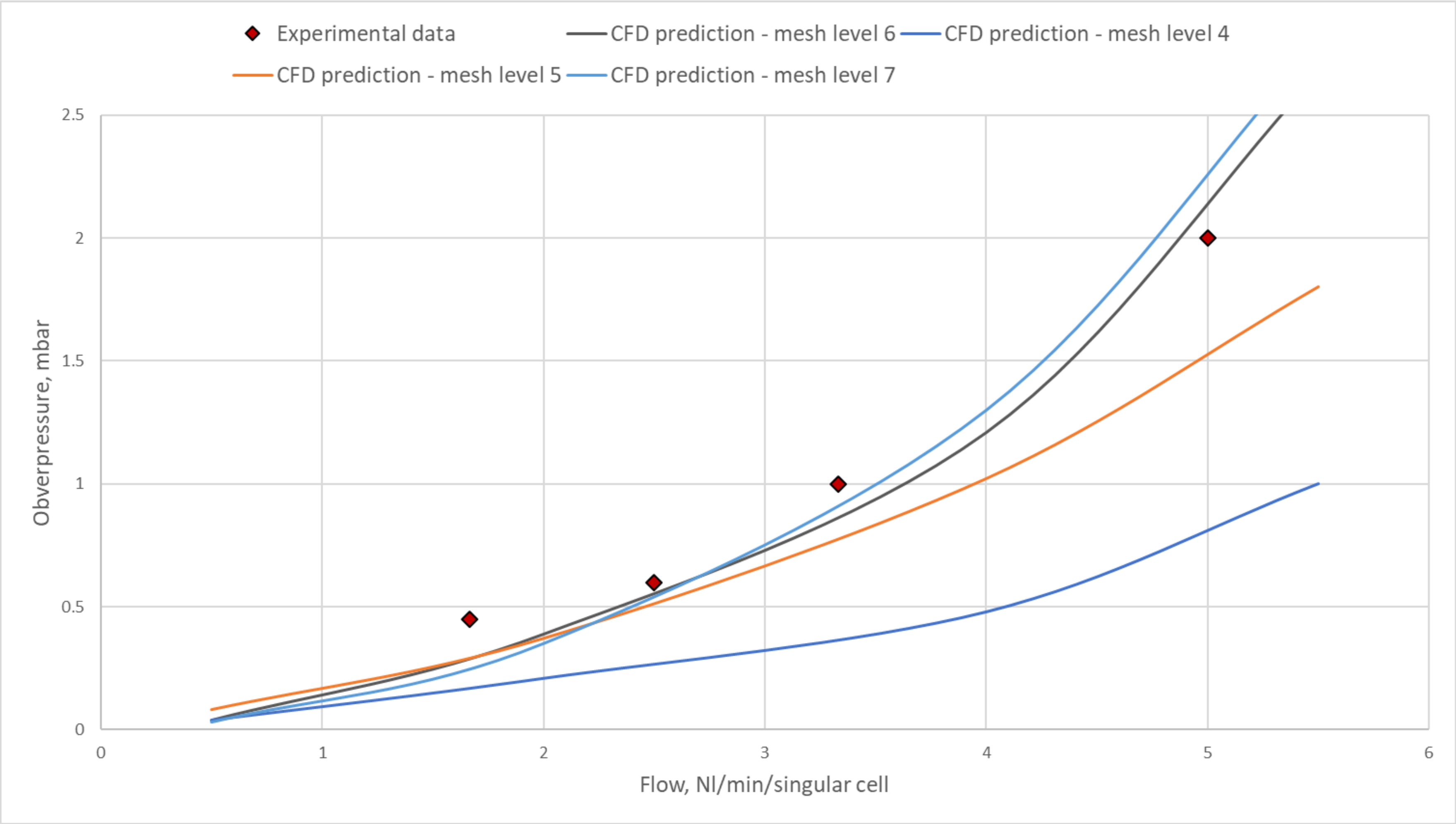


Experimental set-up used to test pressure drop in MCFC stack

A 5kW MCFC stack, used as a reference for CFD model and validation

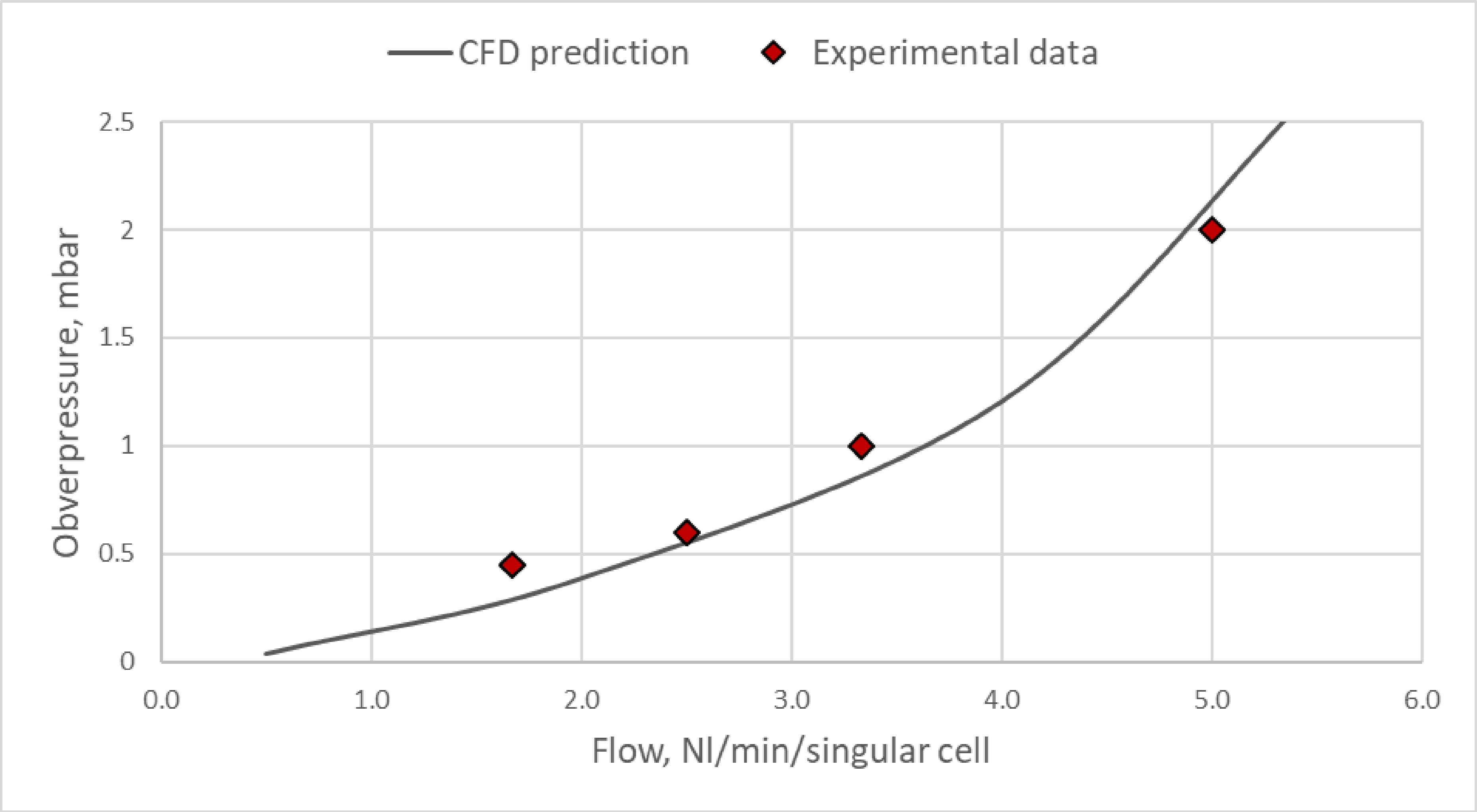
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.3: Computational fluid mechanics (CFD) model



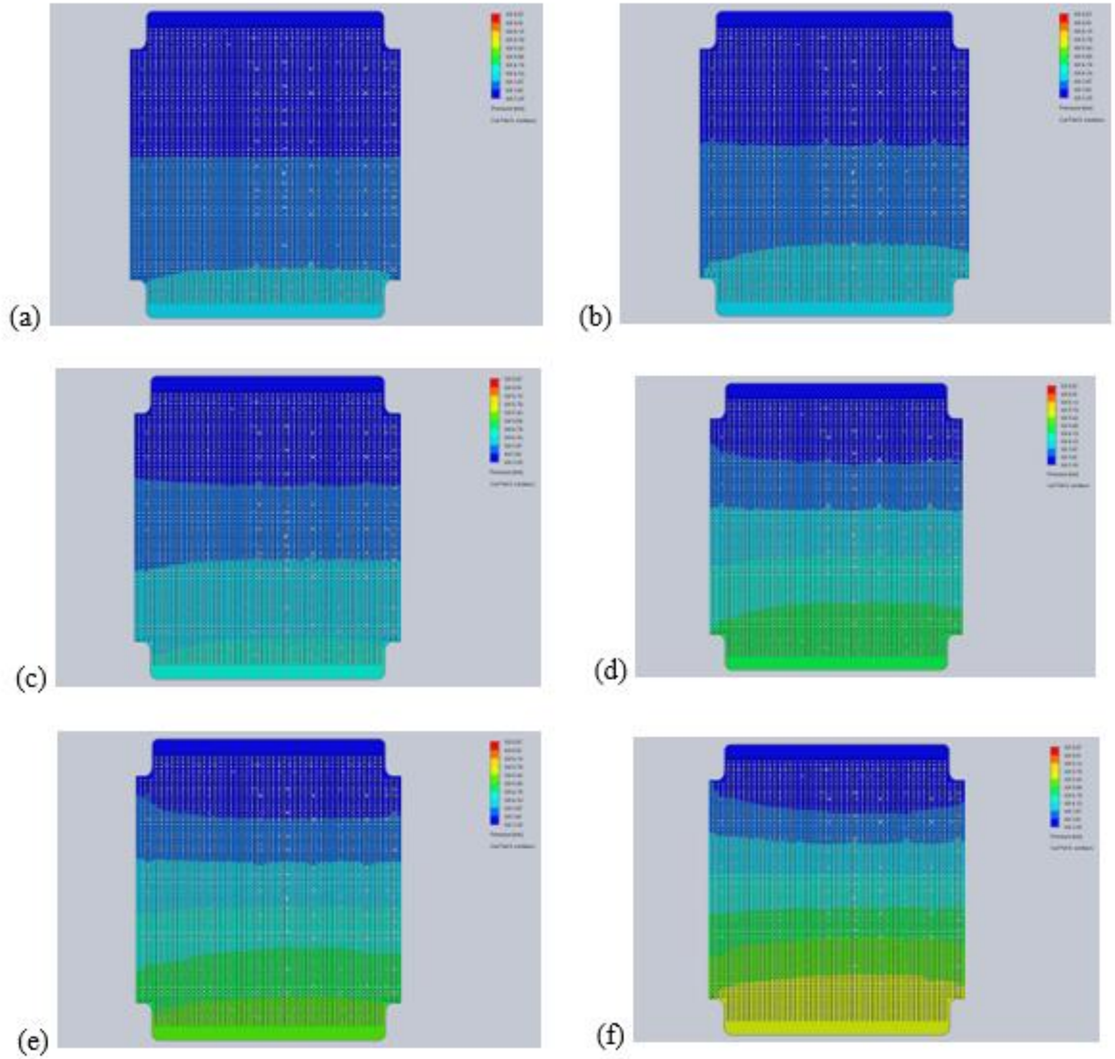
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.3: Computational fluid mechanics (CFD) model



„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Task 2.3: Computational fluid mechanics (CFD) model



0.5 Nl/min: a) 450°C, b) 500°C, c) 650°C
2.0 Nl/min: d) 450°C, e) 500°C, f) 650°C

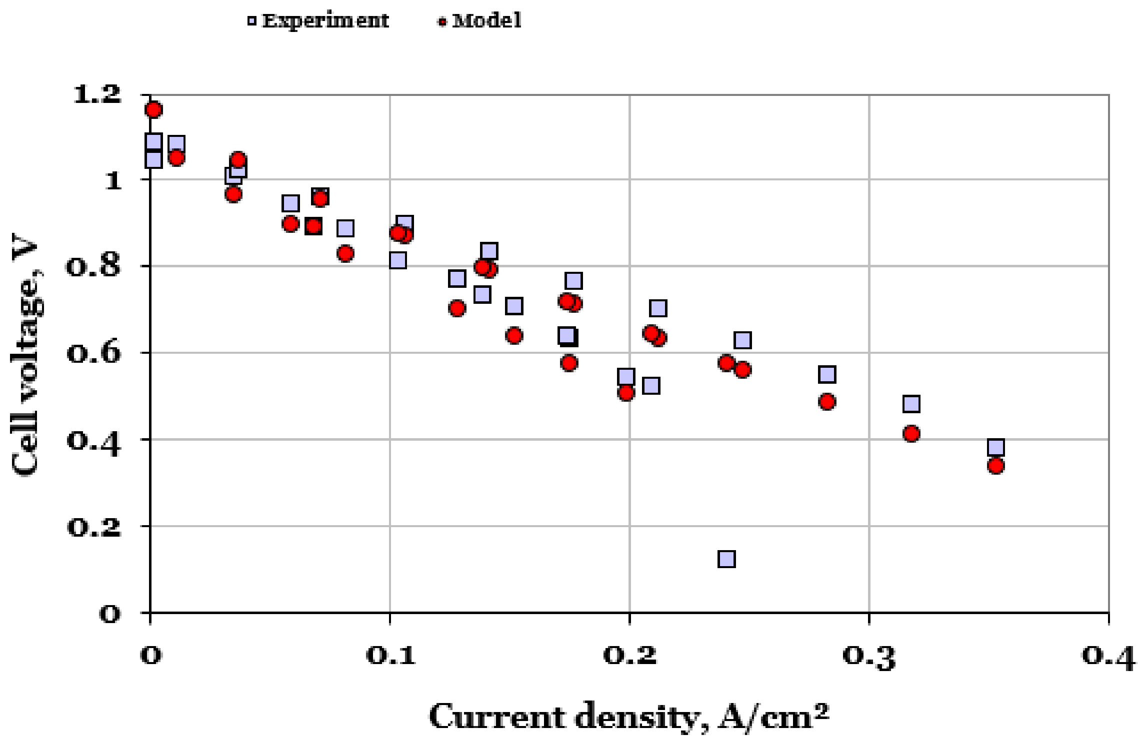
„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

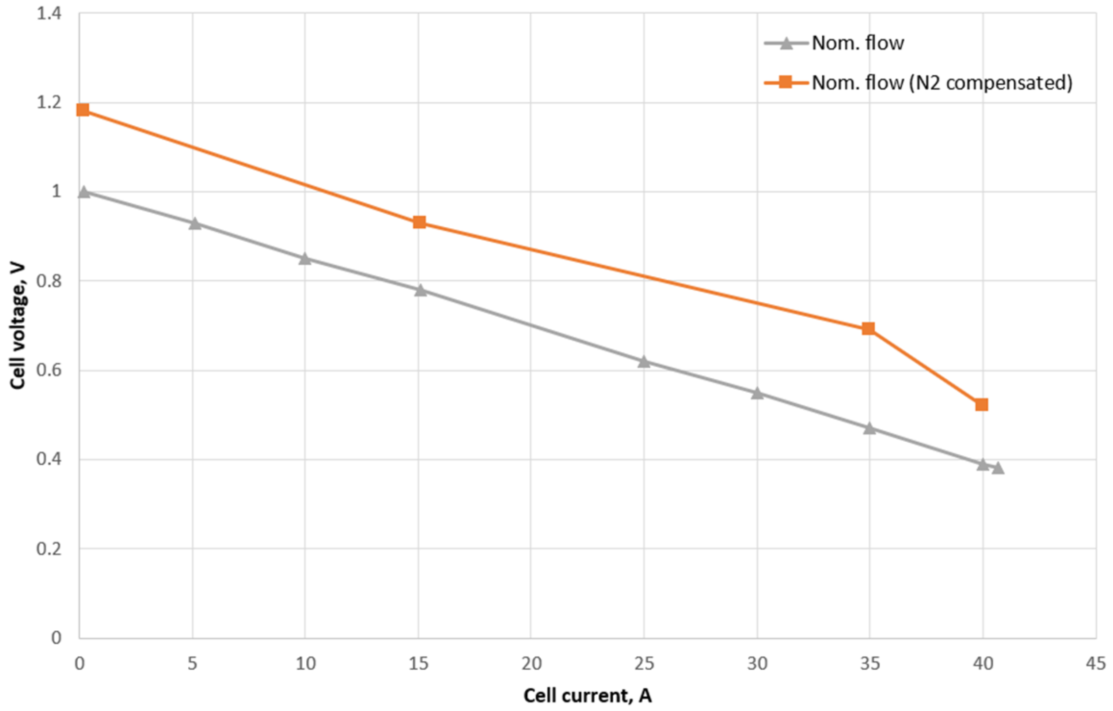
Norway grants

The National Centre for Research and Development

Warsaw University of Technology

Task 2.4: Tuning and validation of a parametric model of the installation from the MCFC





„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00

Norway grants

The National Centre for Research and Development

Warsaw University of Technology

Task 2.5: Verification of assumptions and optimization of operating parameters

A	B	C	D	E	F
Optimum	49.75	10.90	3.564		
MCFC Power	-0.93 kW	-1.00 kW			
MCFC temp	647.58 C	650.00 C		643.37 C	643.37 C
eta_CO2	2.765	41.6231 kg/h	42.8067 kg/h	2.815	4.000
MCFC efficiency	49.97	0.50 kW	50.00		
eta_f	0.94 kW				
m_fuel	0.00 kg/s	2.495e-004	59.87 kg/s		
m_flue gas	0.18 kg/s	1.944	466285.83 kg/s		
				0.3000	
		eta_f [-]	0.66 kW	0.94 kW	0.9900
i_max, MCFC	0.01 kW	i_max [A/cm2]	450.36 C	643.37 C	836.39 C
		Flue gas to MCFC	0.13 kg/s	0.18 kg/s	0.23 kg/s
E_MCFC	0.66 kW	Flue gas to MCFC	0.00 kg/s	0.00 kg/s	0.00 kg/s
number of cell	200.03 kW	Fuel	<empty>	<empty>	<empty>
	200.0				

„Modular system based on Molten Carbonate Fuel Cells with tailored composite members designed for specific flue gas compositions oriented into CCS integration with an industrial power plant", project contract number NOR/POLNORCCS/MOLCAR/00-17/2020-00