TFAWS23-ID-7

Thermomechanical deformation analysis of a tubular solid oxide steam electrolysis cell

Victoria Kurushina, Vinooth Rajendran,
Anil Prathuru, Mamdud Hossain, Nadimul Faisal
School of Engineering, Robert Gordon University,
Aberdeen, AB10 7GJ, UK

Ajith Soman, Bahman Amini Horri, Qiong Cai
University of Surrey, University Campus, Guildford,
GU2 7XH, UK

Thermal & Fluids Analysis Workshop TFAWS 2023
August 21-25, 2023
NASA Goddard Space Flight Center College Park, MD

Contents

- Introduction to solid oxide steam electrolysis (SOE)
  - Solid oxide electrolysis explained
  - Water electrolysis technologies
  - SOE efficiency and advantages
  - SOE integration
  - SOE modelling
  - SOE cell designs
- Project overview
  - Objectives
  - Work packages
  - METASIS experimental tests
- Thermomechanical model
  - Tubular cell design and composition
  - Model set-up
- Results
  - Stress analysis for 800 ^{o}C
  - High temperature effects
  - Effect of boundary conditions
  - Effect of porosity
- Summary

Solid oxide steam electrolysis explained

1 Steam supply at high temperature into the gas channel and splitting into ions of oxygen and hydrogen at the cathode

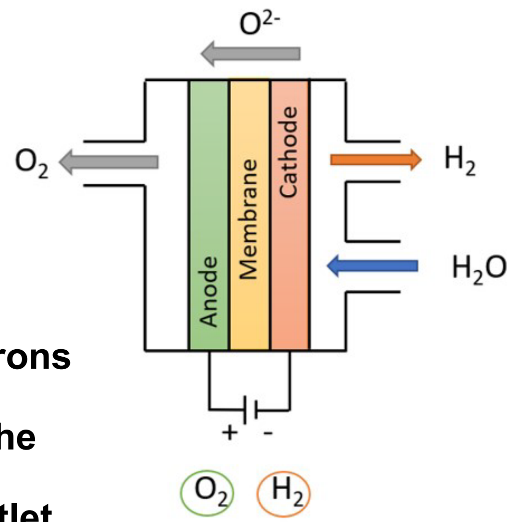
$$H_2O \rightarrow 2H^+ + O^{2-}$$

2 Cations of hydrogen gain electrons at the cathode, powered by the external electrical circuit, and the formed molecules of hydrogen leave the gas channel at the outlet, mixed with the remainder steam

$$2H^+ + 2e^- \rightarrow H_2$$

3 Anions of oxygen pass through the electrolyte (membrane/solution), attracted by the anode, where they loose extra electrons and form zero-valence molecules that exit the gas channel

$$O^{2-} - 2e^- \rightarrow O_2$$



Uses of H_2?

- 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

Uses of O_2?

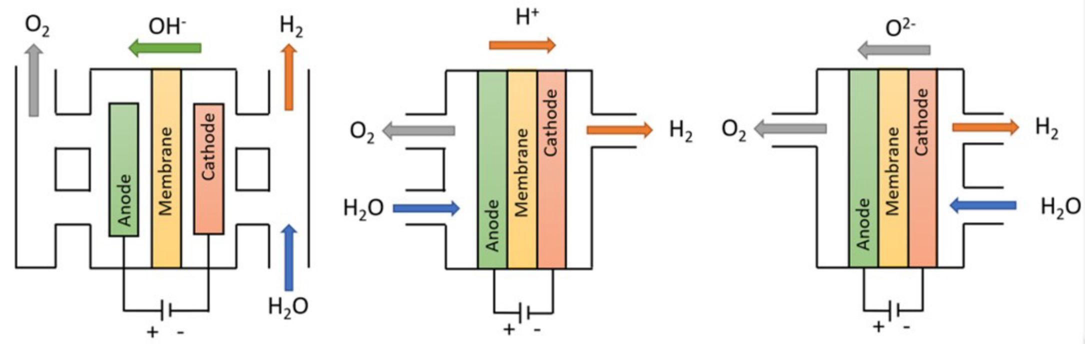
- Part of breathable air for life support
- As oxidizer, for propulsion, welding, cutting
- For medical applications

Introduction to SOE

Water electrolysis technologies

Dominant technologies:

- ***proton exchange membrane electrolysis cells* (PEMEC);**
- **anion exchange membrane electrolysis cells (AEMEC);**
- ***alkaline water electrolysis cells* (AWEC);**
- ***solid oxide steam electrolysis cells* (SOSEC);**
- **thermochemical water splitting (TWS);**
- **photolysis water splitting (PWS);**
- **photoelectrochemical water electrolysis cells (PECWEC).**



PEMEC – mature

AWEC – commercial

SOSEC – demonstration

Characteristics	Units	PEMEC	AEC	SOEC
Operating temperature	°C	50-80	60-80	650-1000
Current density	A/cm^2	0.6-2.0	0.2-0.4	0.3-2.0
Cell voltage	V	1.8-2.2	1.8-2.4	0.7-1.5
Operating pressure	bar	< 200	< 30	< 25
Production rate	m^3/h	< 40	< 760	< 40
Stack lifetime	hours	20 000 - 60 000	60 000 - 90 000	10 000
Stack energy	kWh/m^3	4.2-5.5	4.2-5.9	>3.2
Capital cost	euro/kW	1 860 - 2 320	1 000 - 1 200	> 2 000

SOE efficiency and advantages

- **Higher temperature leads to better performance due to reduction in anode and cathode activation overpotential.**
- **However, it creates thermal stress and less durable cells.**

Current challenges

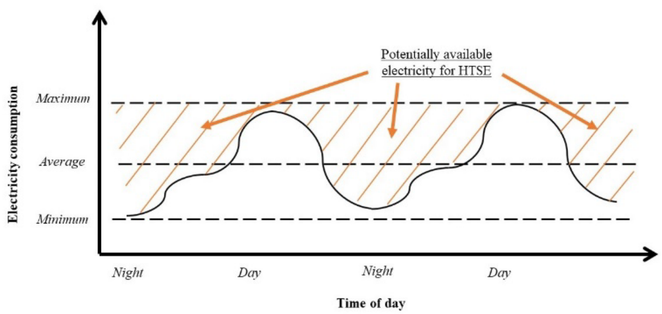
1. **Costs should be reduced for all stages of the stack lifecycle.**
2. **Material degradation accelerated in high temperature conditions.**
3. **Fabrication of cells, production of complex materials may not be completely clean.**
4. **Lack of commercialization.**
5. **Lack of manufacturing innovations.**

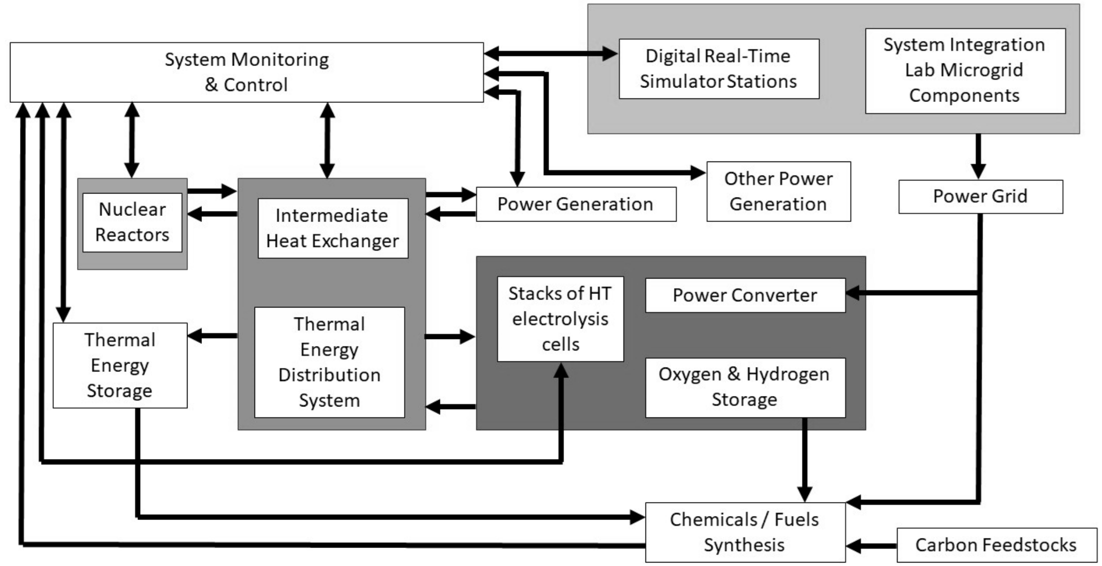
Advantages

1. **High efficiency, achievable in high temperature conditions.**
2. **Combined input of thermal and electrical energy makes it compatible with wide range of systems with either type of excess energy.**
3. **SOEC, SOFC and reversible cells are well suited for intermittent operation.**
4. **Use of solid materials for the functional layers simplifies transportation, installation and operation.**
5. **SOEC operation is environmentally friendly.**

SOE integration

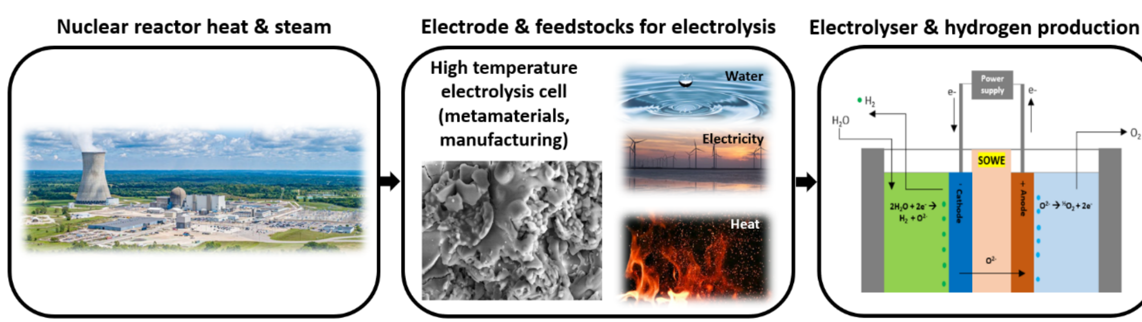
- Heat
- Electricity
- Feedstock materials





Integration potential:

- ❑ Nuclear plants
- ❑ Solar plants
- ❑ Wind farms
- ❑ Hybrid energy systems
- ❑ Aviation
- ❑ Spacecraft systems, etc.



SOE modelling

Black-box models → Grey-box-models → White-box models

Accounting for the physics of the process

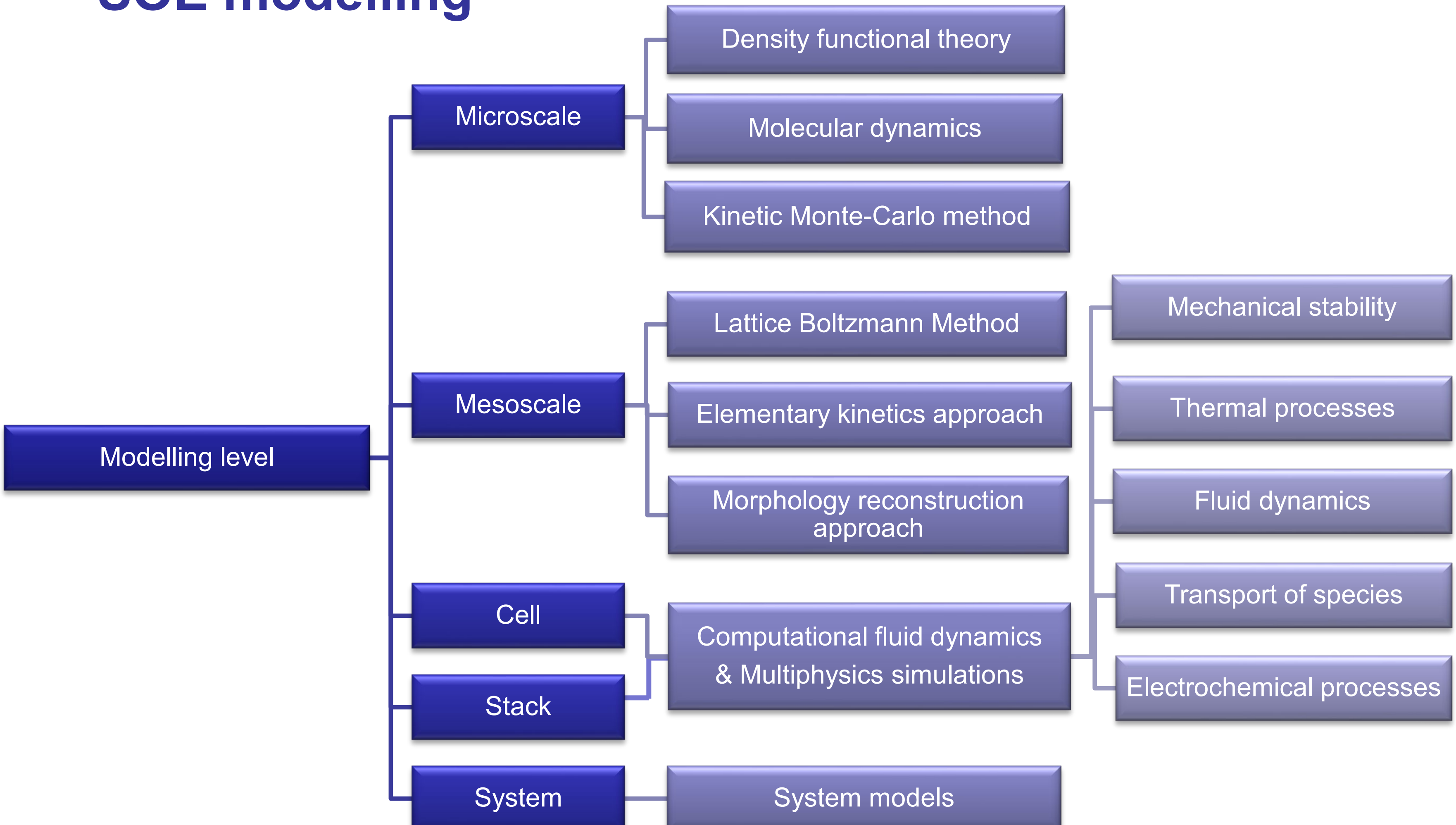
0D → 1D → 2D → 3D

Model dimensionality (spatial)

Steady-state models | Transient models

Model dimensionality (temporal)

SOE modelling



Introduction to SOE

SOE cell designs

Support type

- Cathode-supported cell
- Electrolyte-supported cell
- Anode-supported cell
- Metal-supported cell

Thick cathode

+ Good cell stability during electrochemical process
- High resistance for polarization

Thick electrolyte

+ High mechanical robustness
+ Good gas diffusion properties
- High ohmic losses in the thickened electrolyte layer

Thick anode

+ Lower operating temperature
+ Low ohmic resistance
+ Lower costs of material
+ Considered to be easier for fabrication
- Lower mechanical reliability

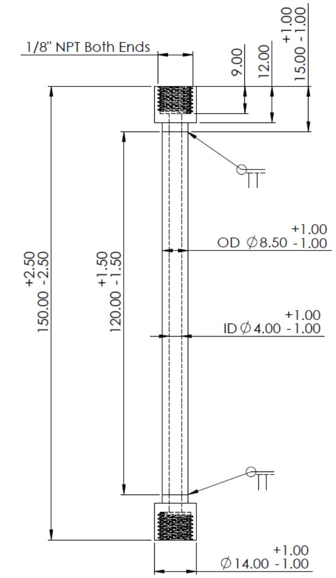
Thick metal

+ High mechanical stability
- Energy losses in the supporting porous metal layer

Project overview

Objectives

- Development of large-scale and hierarchical length scale cathode catalyst layer (tubular metasurface) using thermal spray coating technique (using air plasma spray) for an enhanced structurally stable SOSE cell design;
- Development of a customised SOSE cell design with a tubular electrode assembly for an integration with high temperature steam line (with higher thermo-mechanical and electro-chemical performance and long-term structural stability).



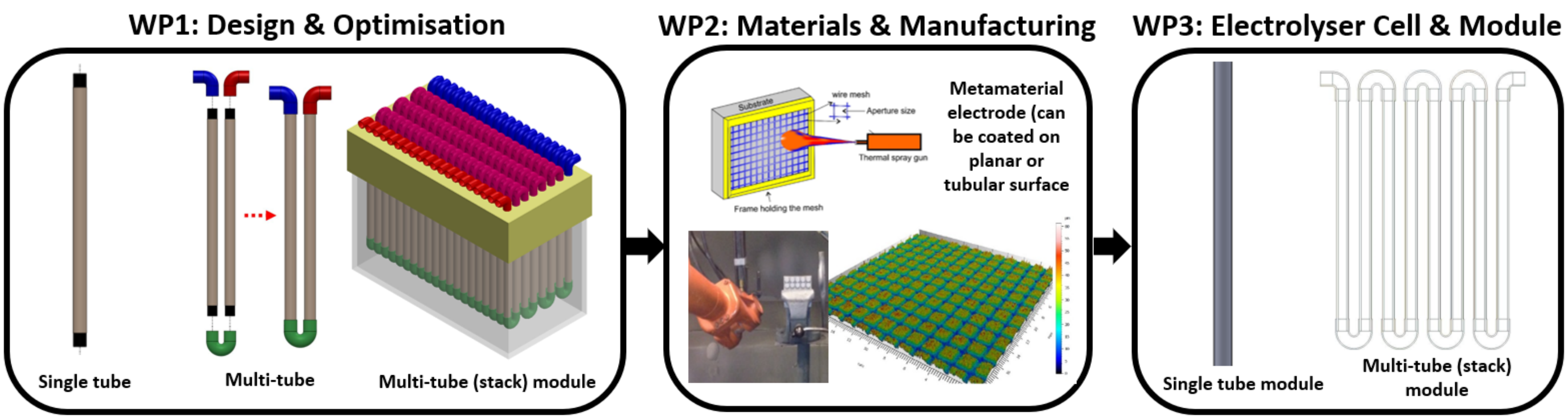
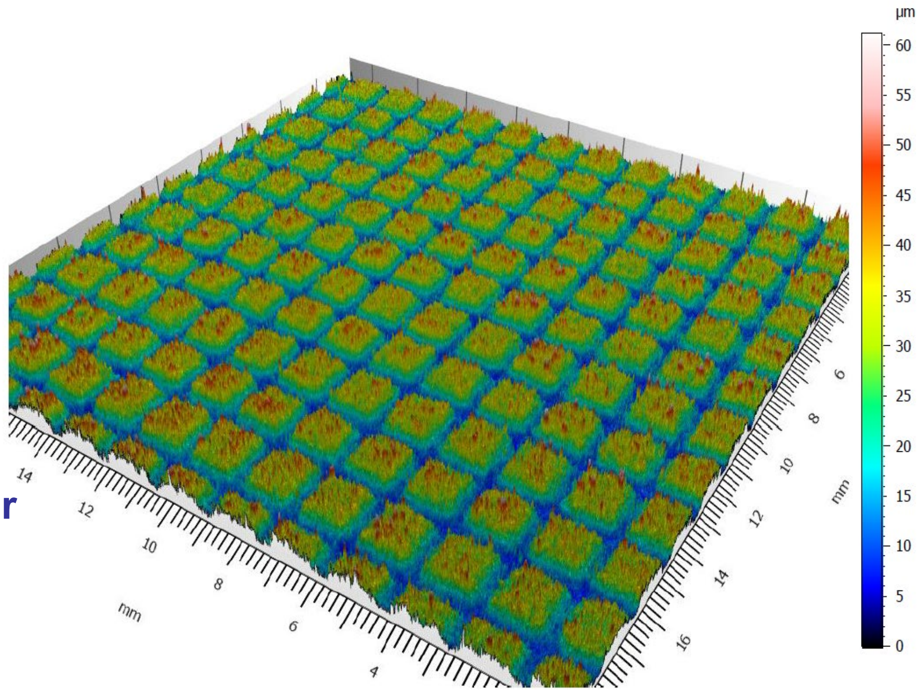


Fig. 1 METASIS methodology.

Work packages

- **WP1 (Electrolyser design and optimisation)**
  - Task 1.1. Benchmarking of electrolyser
  - Task 1.2. Structural analysis
  - Task 1.3. Computational fluid dynamics
- **WP2 (Materials selection, manufacturing, and electrode cell development)**
  - Task 2.1 Materials selection and processing
  - Task 2.2. Electrode materials comparison
- **WP3 (Scaled manufacturing of electrolyser cell with metasurface design)**
  - Task 3.1. Manufacturing of tubular electrode with metasurface cathode
  - Task 3.2. Prototype testing and validation

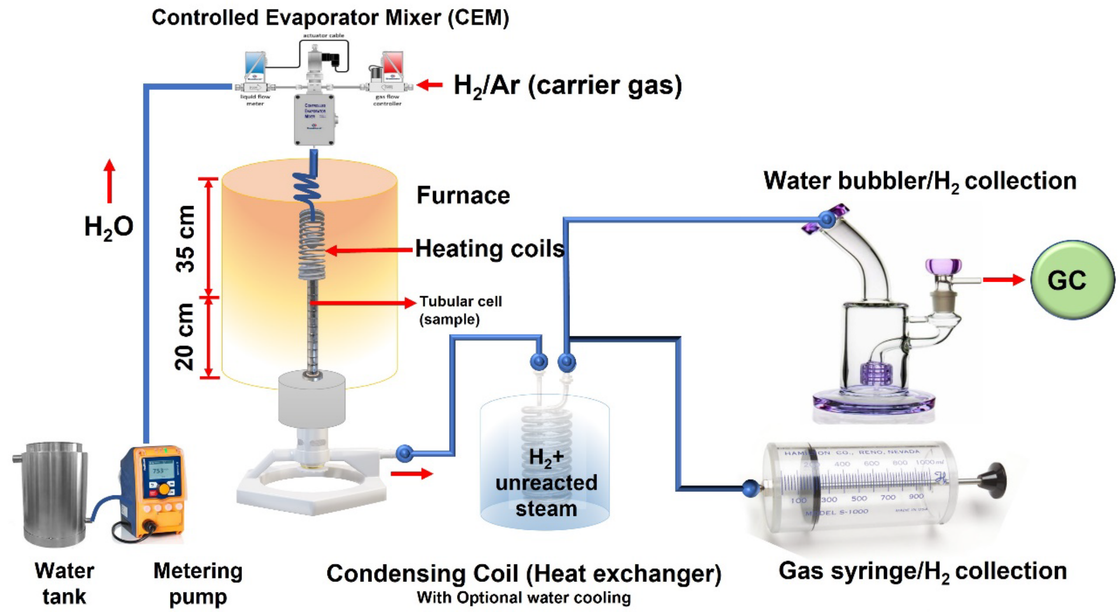


METASIS experimental tests

Our targets

- Improving efficiency
- Lower cost
- Durability
- Scalability & system integration

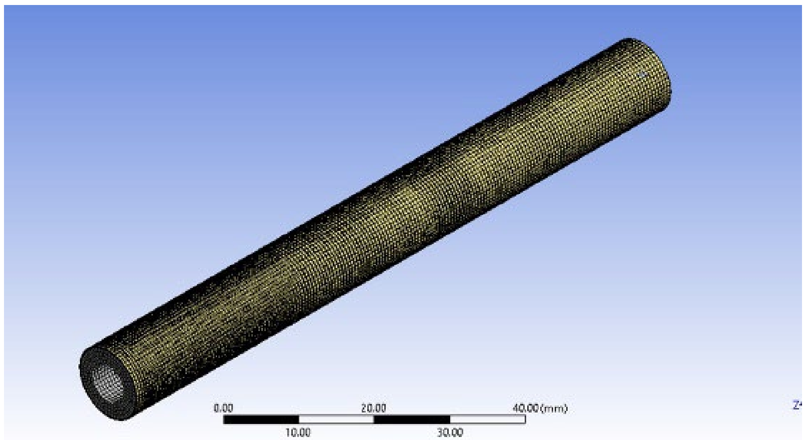
<u>Material characterization</u> tests to be performed in the Robert Gordon University

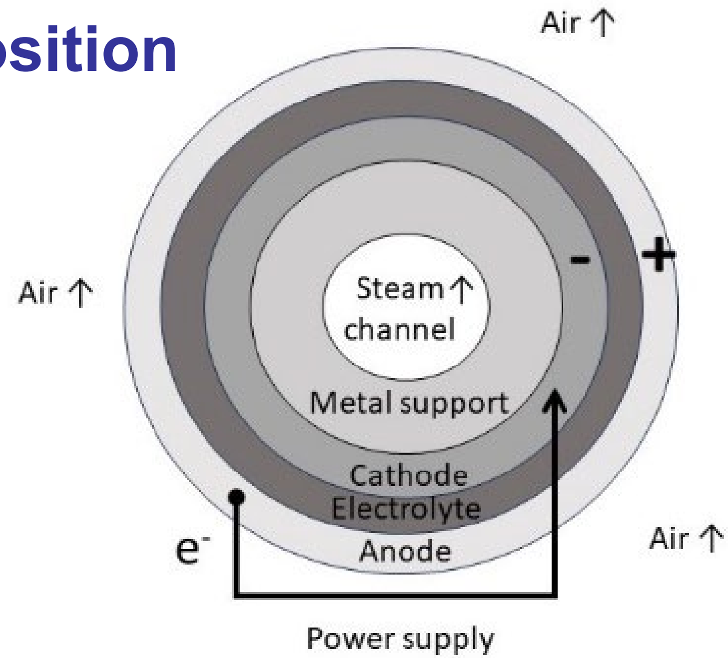


<u>High temperature</u> tests to be performed in the University of Surrey

Thermomechanical model

Tubular cell design and composition





Layer	Functionality	Thickness (per design), mm	Material	Proposed manufacturing technique	Porosity (per design), %
1	Substrate	2.150	Titanium alloy	Commercial	30
2	Interconnect	0.035	Silver	Electrodeposition	0
3	Cathode	0.070	Nickel oxide and GDC	Dip coating / Thermal spray	30
4	Electrolyte	0.022	GDC and YSZ	Dip coating	0
5	Anode	0.070	GDC and LSCF	Dip coating / Thermal spray	30
6	Interconnect	0.035	Silver	Wire wrapped around the cell	30

Thermomechanical model

Tubular cell design and composition

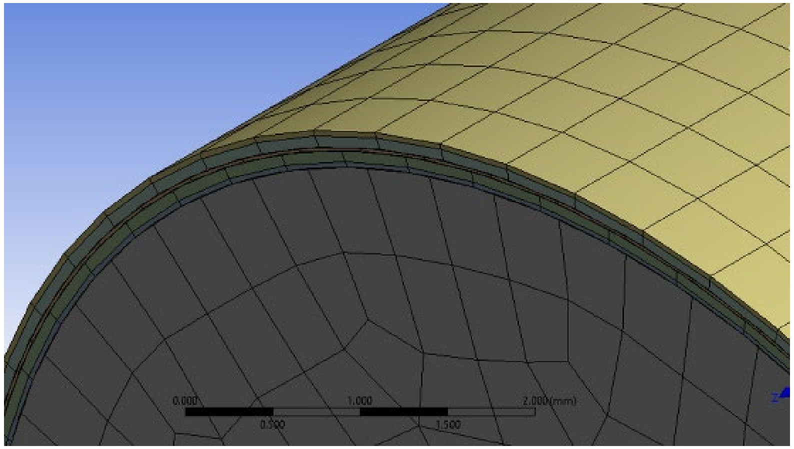
Material	Density, kg/m³	Melting temperature, °C	Young's modulus, GPa	Poisson ratio	Thermal expansion coefficient, µm/m·°C	Tensile yield strength, MPa	Ultimate yield strength, MPa
Titanium alloy	4405	1370	107	0.32	8.9	850	1098
Silver	10500	961	83	0.37	19	54	140
Nickel oxide	4670	1605	160	0.26	12.5	440	646
GDC	7200	2600	120	0.26	11.5	1.95	200
YSZ	5900	2700	210	0.28	10.5	750	1200
LSCF	6000	920	170	0.30	14.5	94	160

Property	Units	Cathode	Electrolyte	Anode
Density	kg/m³	5682	7082	6600
Melting point	°C	2003	2609	1760
Young's modulus	GPa	144	128	145
Poisson's ratio		0.26	0.26	0.28
Thermal expansion coefficient	µm/m·°C	12.1	11.4	13
Tensile yield strength	MPa	265	24.5	48
Ultimate yield strength	MPa	467	223	180

Thermomechanical model

Model set-up

- **Standard solid elements for the substrate**
- **Shell elements for five functional layers**
- **Full tube of 100 mm length and 6 mm internal diameter**
- **Bonded contacts set between the layers**
- **The sixth layer is assumed to be a layer of a uniform material**



#	Number of cells	Maximum total deformation of the outer silver interconnect, mm	Maximum total deformation of the titanium substrate, mm
1	22 537	0.10441	0.079562
2	37 862	0.11159	0.078981
3	50 962	0.11234	0.078593
4	76 192	0.11036	0.078641
5	**90 762**	**0.088686**	**0.078468**
6	118 342	0.094807	0.078269
7	129 009	0.087868	0.079190
8	141 911	0.089302	0.078229

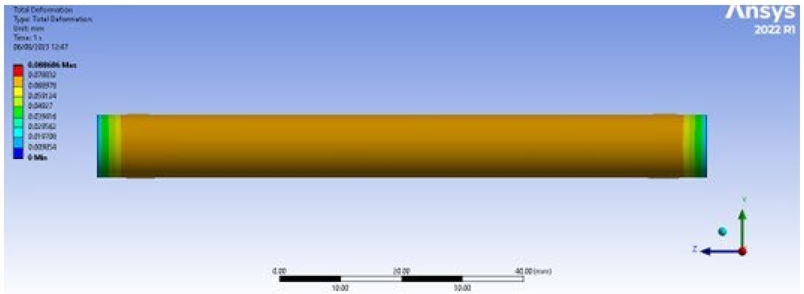
Base case == worst case of the thermal expansion in the middle of the temperature range:

- **Fixed-fixed connections**
- **No porosity**
- **800 °C thermal load**
- **1 MPa internal pressure**

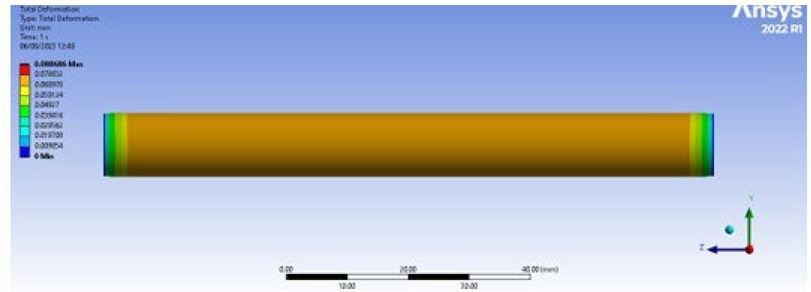
Results

Stress analysis for 800 °C

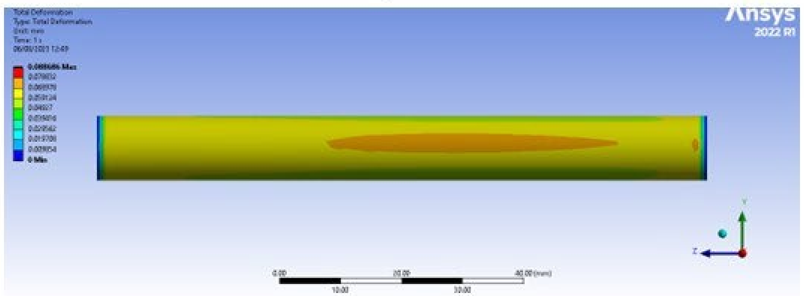
- View from the X axis
- Fixed-fixed boundary conditions



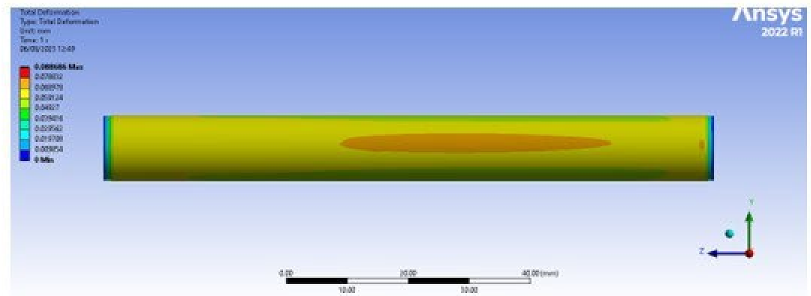
Layer 1



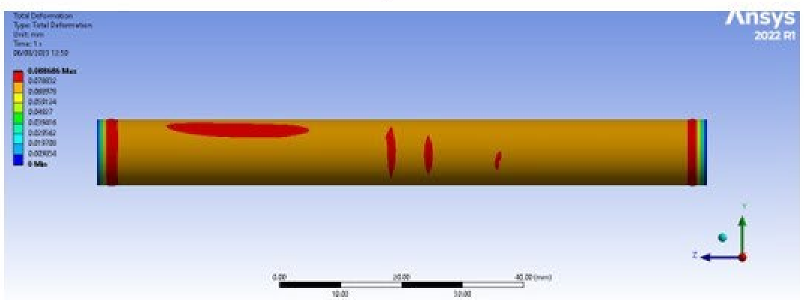
Layer 2



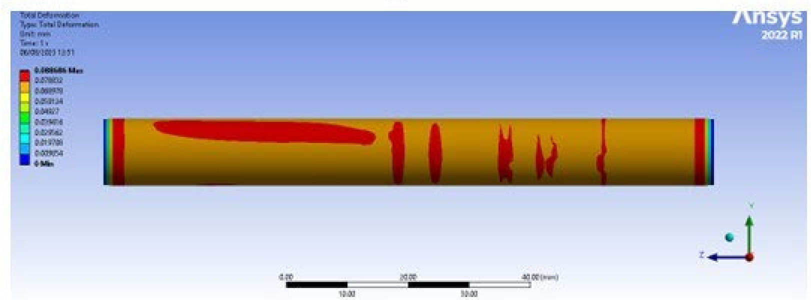
Layer 3



Layer 4



Layer 5

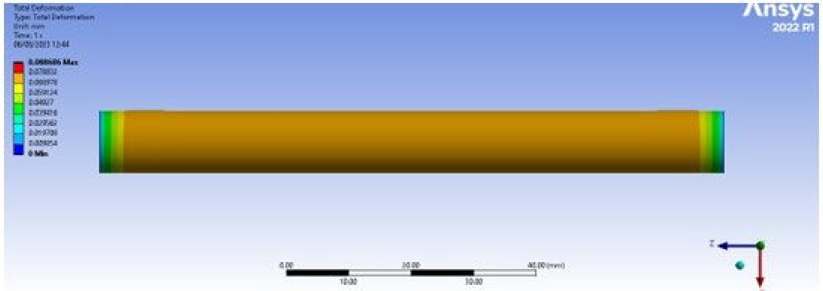


Layer 6

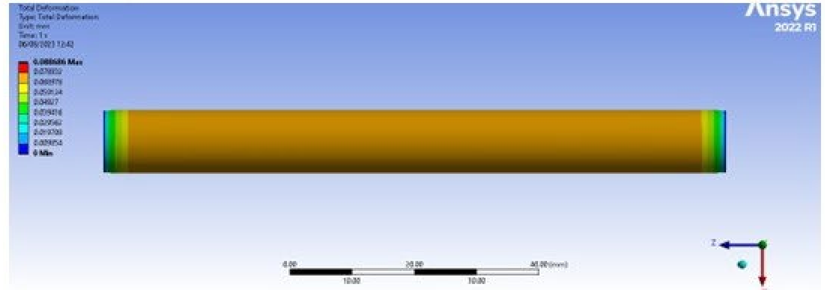
Results

Stress analysis for 800 °C

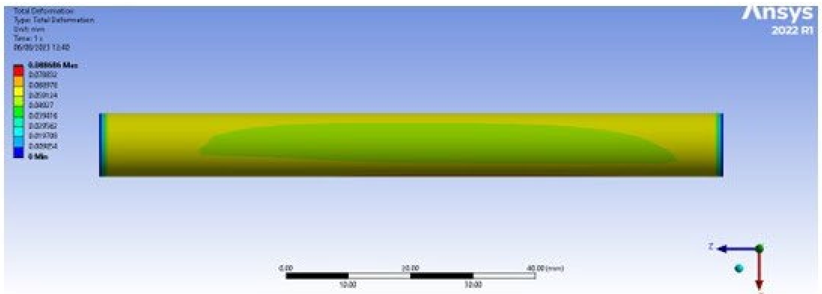
- View from the Y axis
- Fixed-fixed boundary conditions



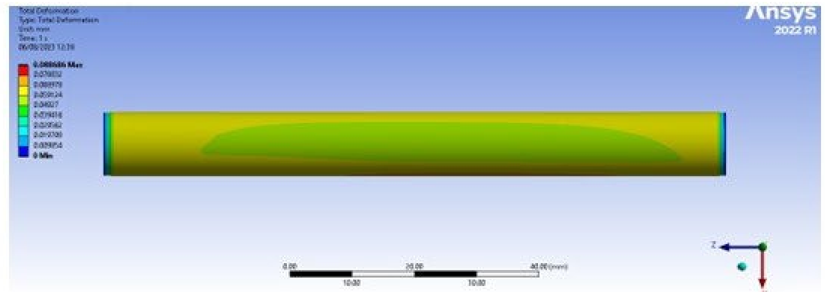
Layer 1



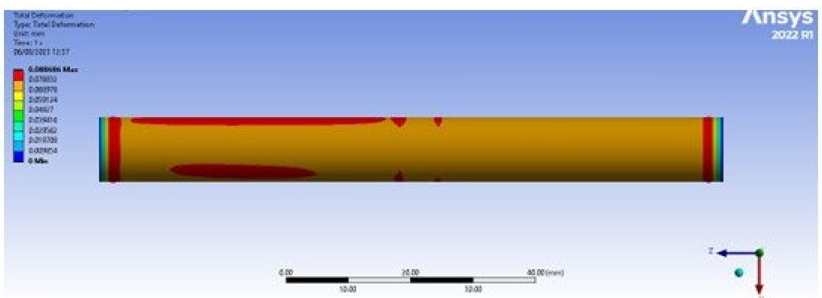
Layer 2



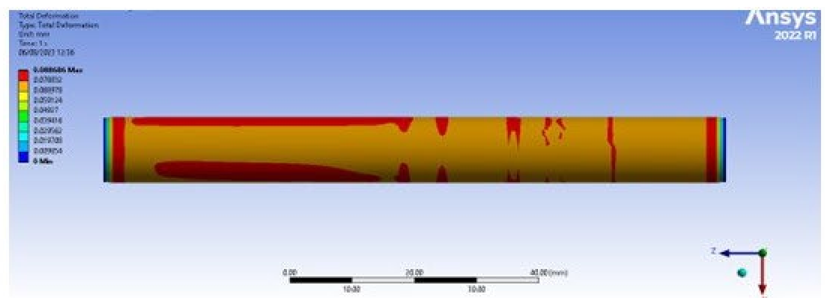
Layer 3



Layer 4



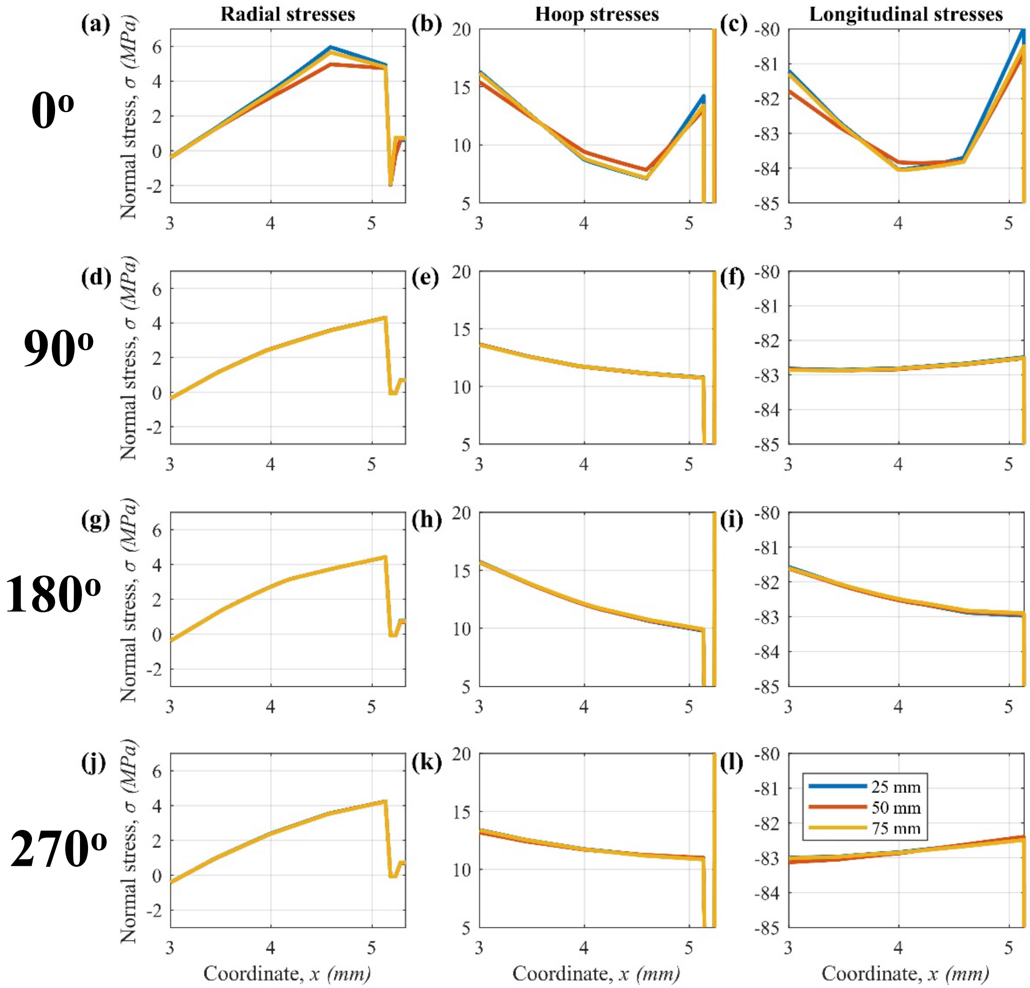
Layer 5



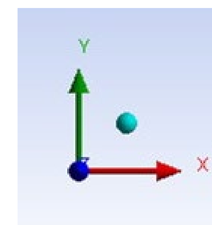
Layer 6

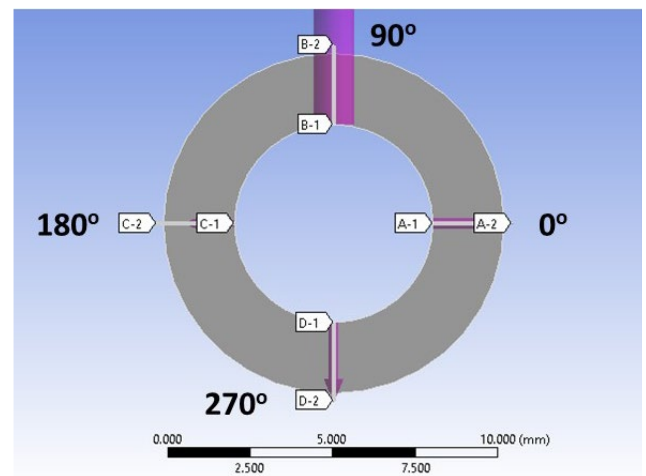
Results

Stress analysis for 800 °C



- Normal stresses observed with fixed-fixed boundaries – enlarged for comparison

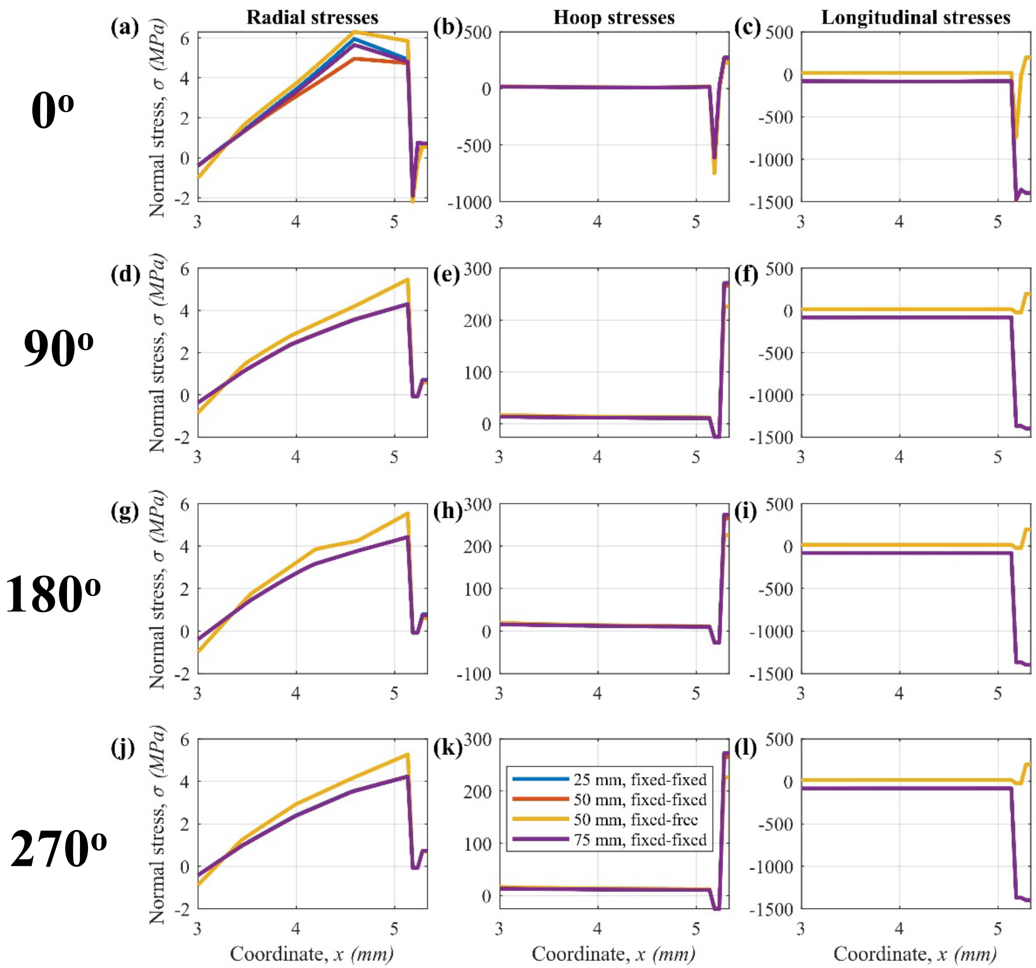




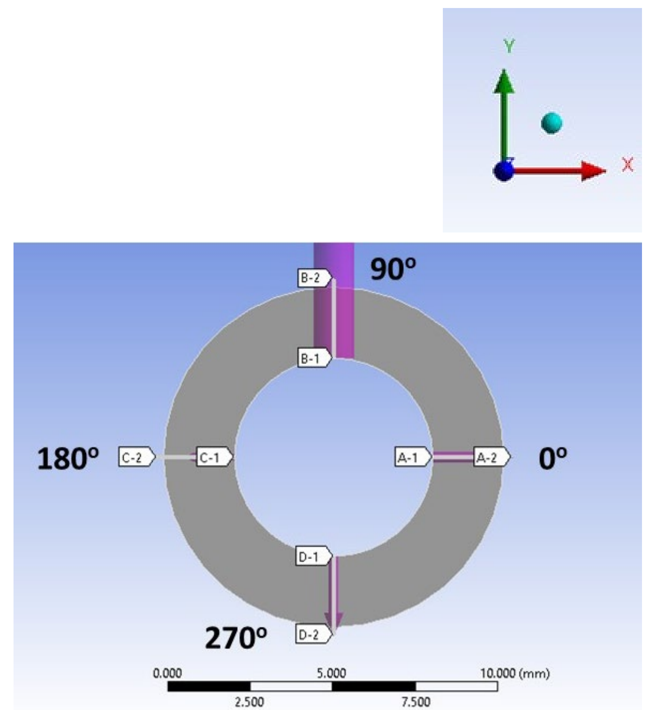
Orientation cross-section cuts

Results

Effect of boundary conditions



- Normal stresses in comparison for fixed-fixed and fixed-free boundary conditions – full scale

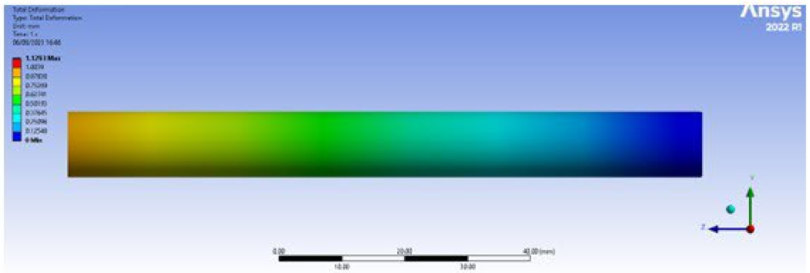


Orientation cross-section cuts

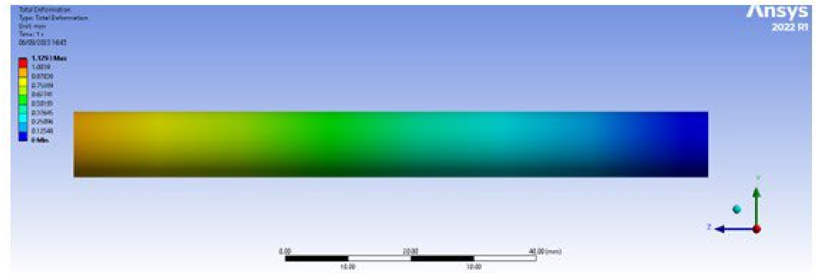
Results

Effect of boundary conditions

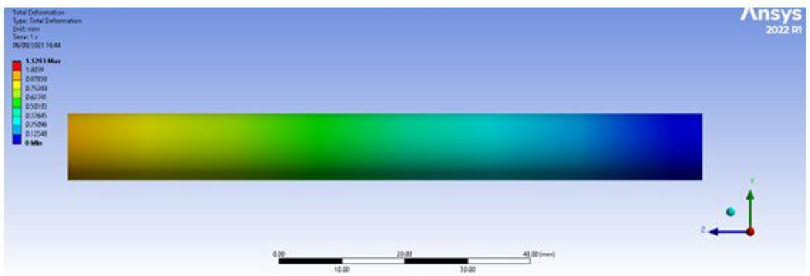
- ➢ **Total deformation at fixed-free conditions**
- ➢ **Temperature 800 °C**



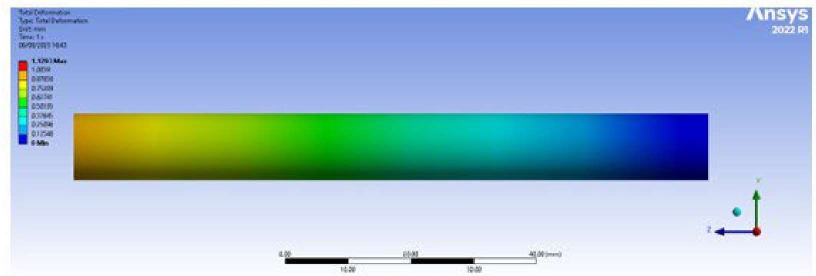
Layer 1



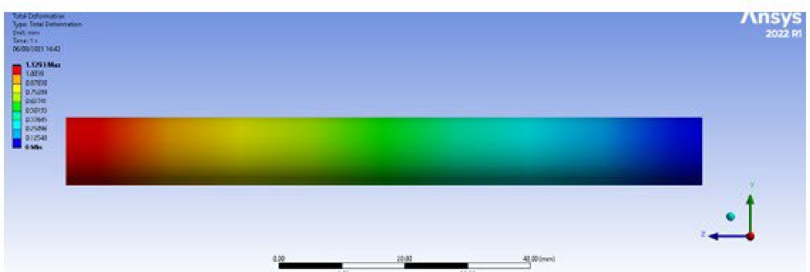
Layer 2



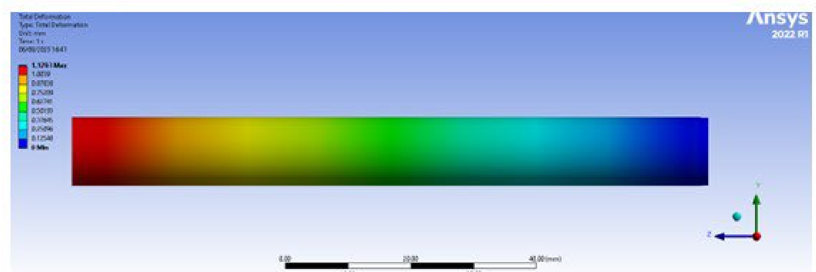
Layer 3



Layer 4



Layer 5

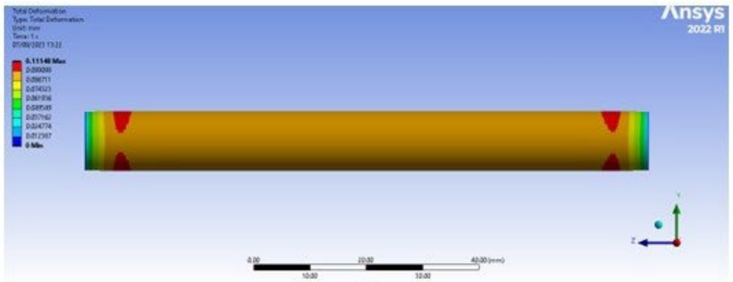


Layer 6

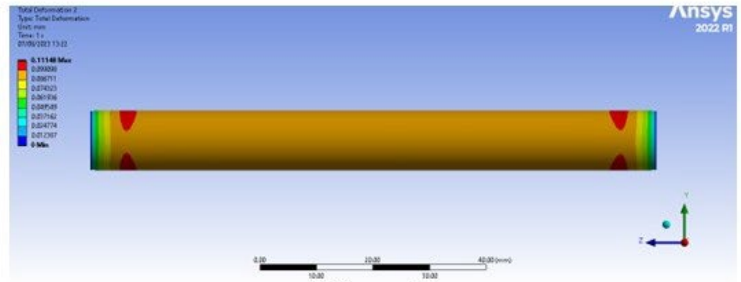
Results

High temperature effects

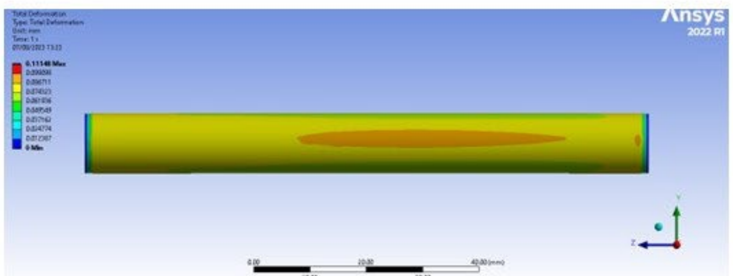
- View from X axis
- Temperature 1000 ^{o}C
- Fixed-fixed boundary conditions



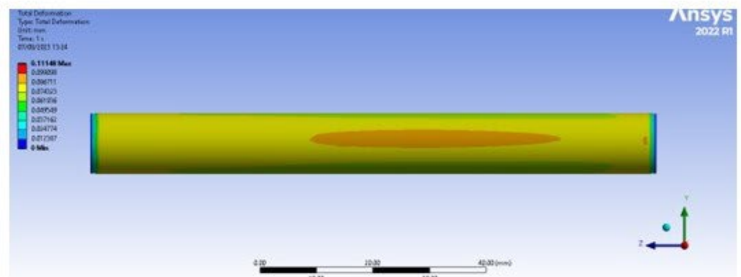
Layer 1



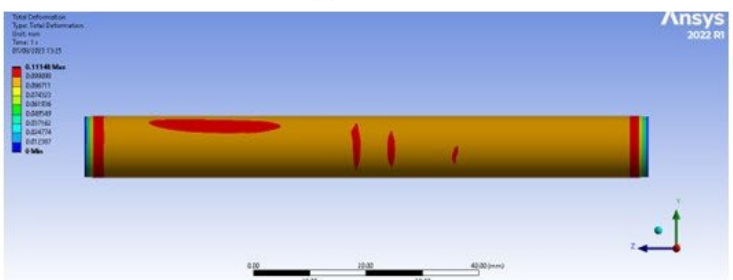
Layer 2



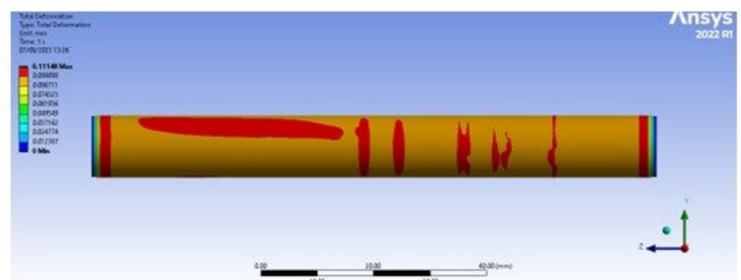
Layer 3



Layer 4



Laver 5

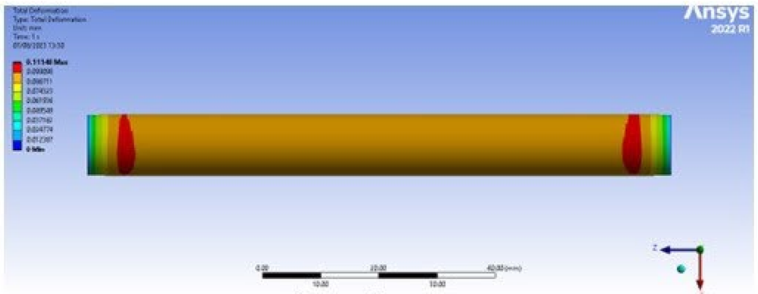


Layer 6

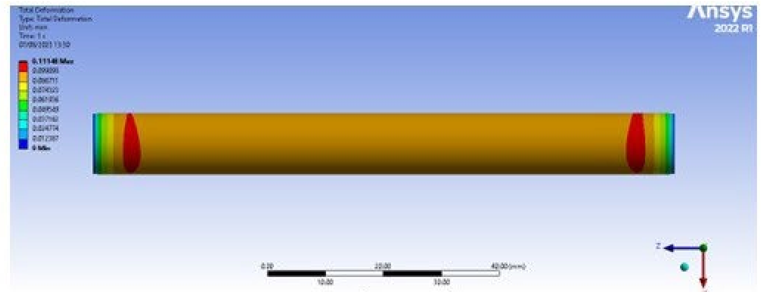
Results

High temperature effects

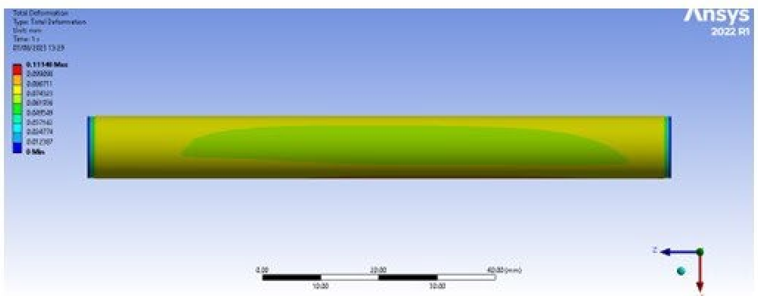
- View from Y axis
- Temperature 1000 °C
- Fixed-fixed boundary conditions



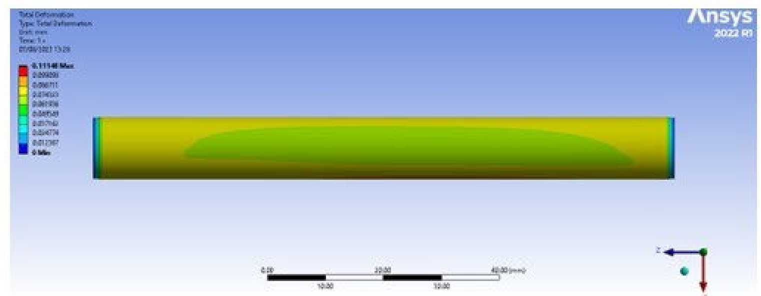
Layer 1



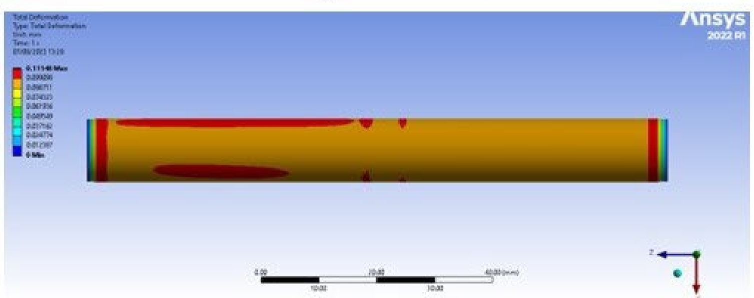
Layer 2



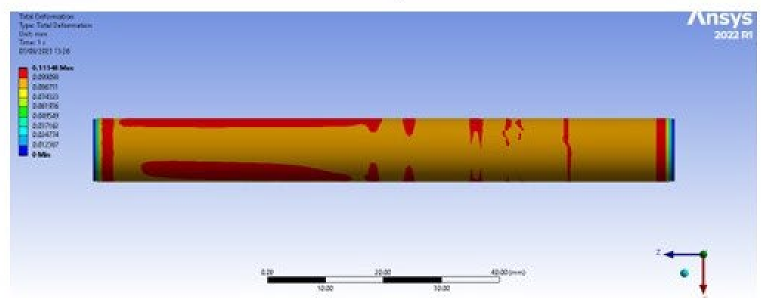
Layer 3



Layer 4



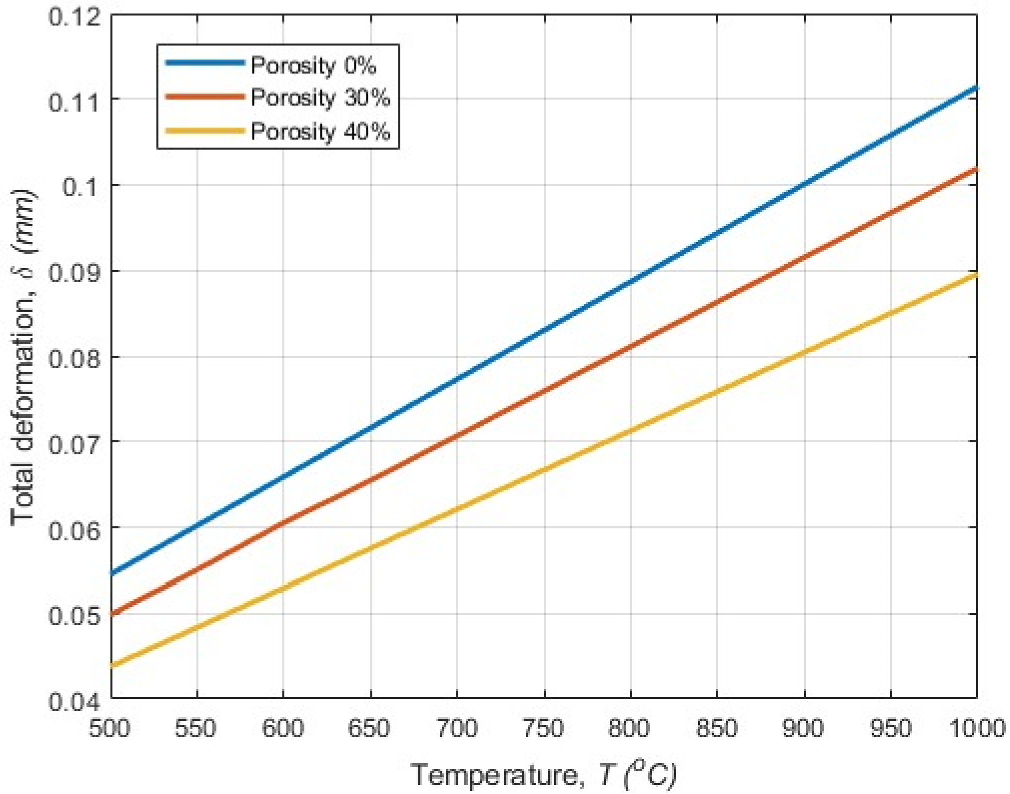
Layer 5



Layer 6

High temperature effects

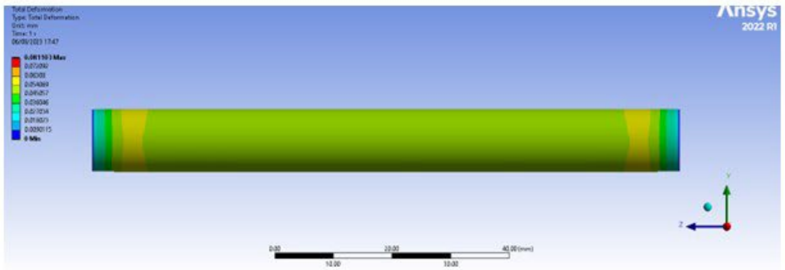
Deformation of the outer layer



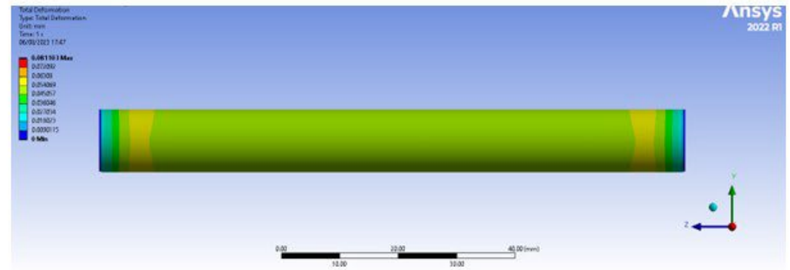
Results

Effect of porosity

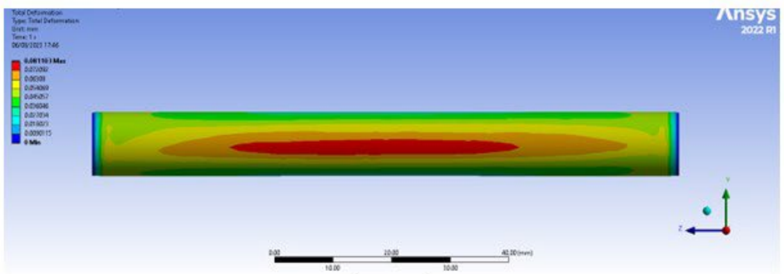
- **Total deformation with the designed 30 % porosity in layers 1, 3, 5, 6**
- **Temperature 800 ^{o}C**



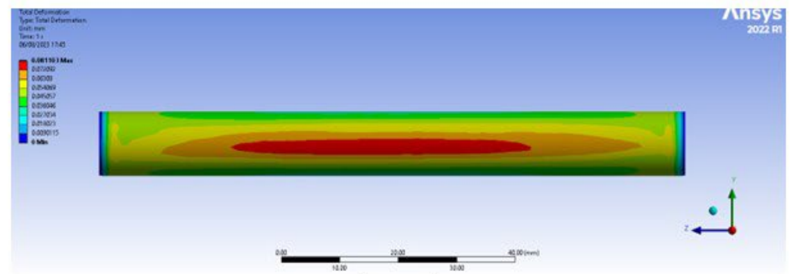
Layer 1



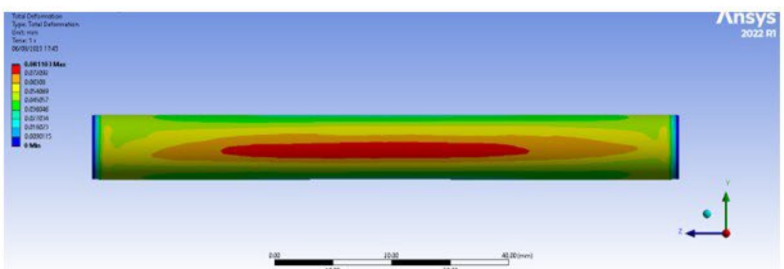
Layer 2



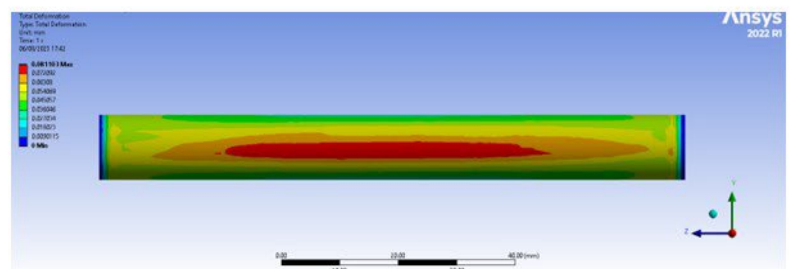
Layer 3



Layer 4



Layer 5

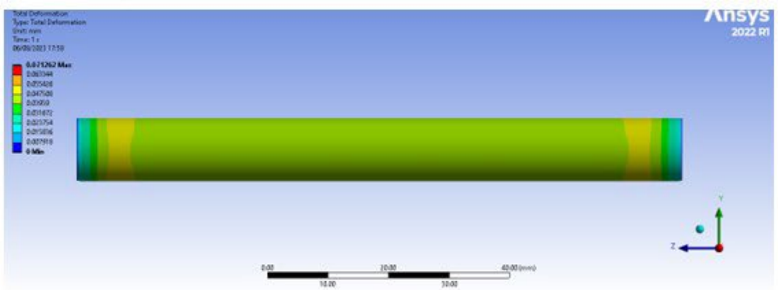


Layer 6

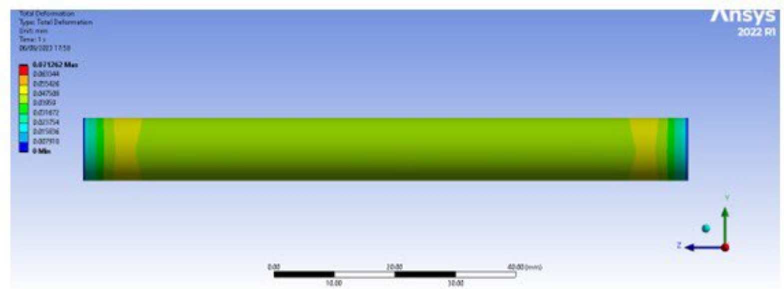
Results

Effect of porosity

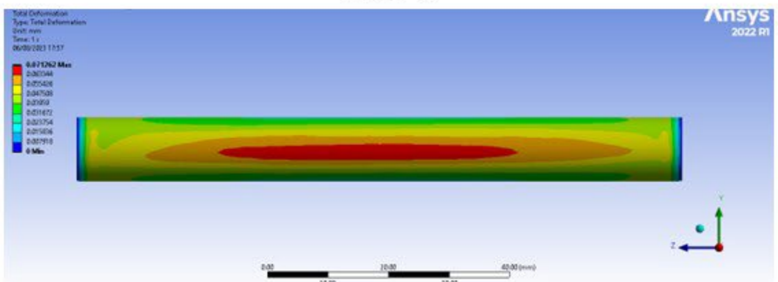
- Total deformation with the 40 % porosity in layers 1, 3, 5, 6
- Temperature 800 °C



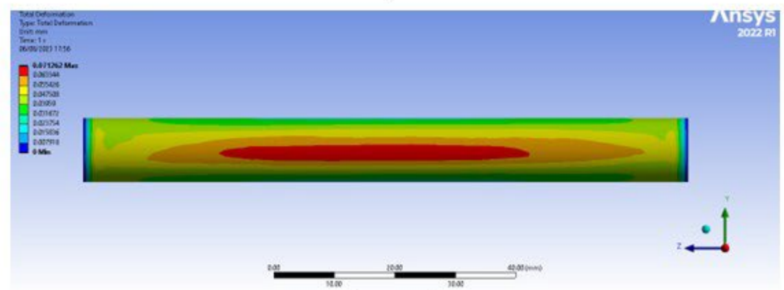
Layer 1



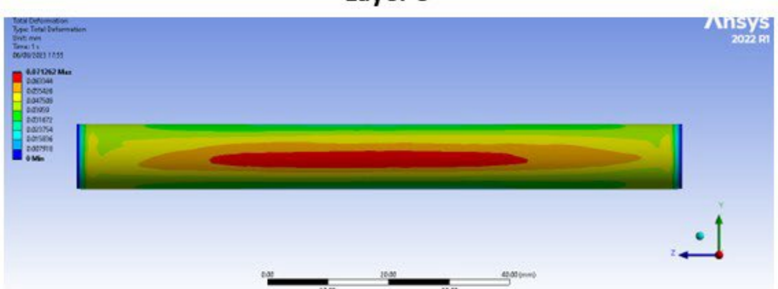
Layer 2



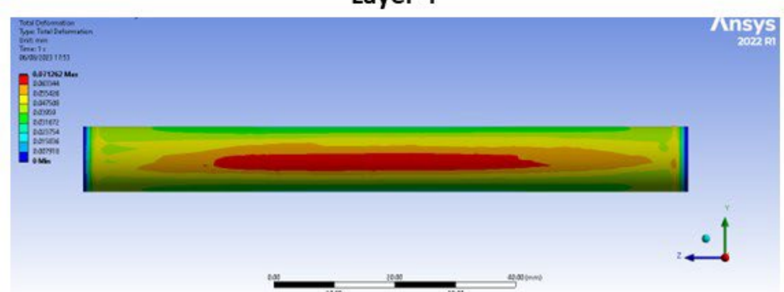
Layer 3



Layer 4



Layer 5



Layer 6

Summary

Conclusions:

- ❑ Identified areas of potential crack occurrence and delamination.
- ❑ Important impact of the difference in the CTE among the layers.
- ❑ Total deformation increases about 1.4 times with the temperature growth from 600 to 800 ^{o}C for the non-porous structure.
- ❑ Increase in porosity from 30% to 40% may lead to approximately 10% reduction in the total deformation.

Next steps:

❑ Electrochemistry and fluid dynamics analysis, accounting for the thermomechanical deformation.

❑ Benchmarking with the high temperature SOEC tests in the laboratory.

Thank you

Please, feel free to get in touch:

Professor Nadimul Faisal (RGU) n.h.faisal@rgu.ac.uk

Dr Victoria Kurushina (RGU) v.kurushina@rgu.ac.uk, v.kurushina@outlook.com

ROBERT GORDON UNIVERSITY ABERDEEN

Engineering and Physical Sciences Research Council

UNIVERSITY OF SURREY