NASA Johnson Space Center
Thermal and Fluids Analysis Workshop

Solid Oxide CO_2 Electrolysis Technical Overview

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Overview

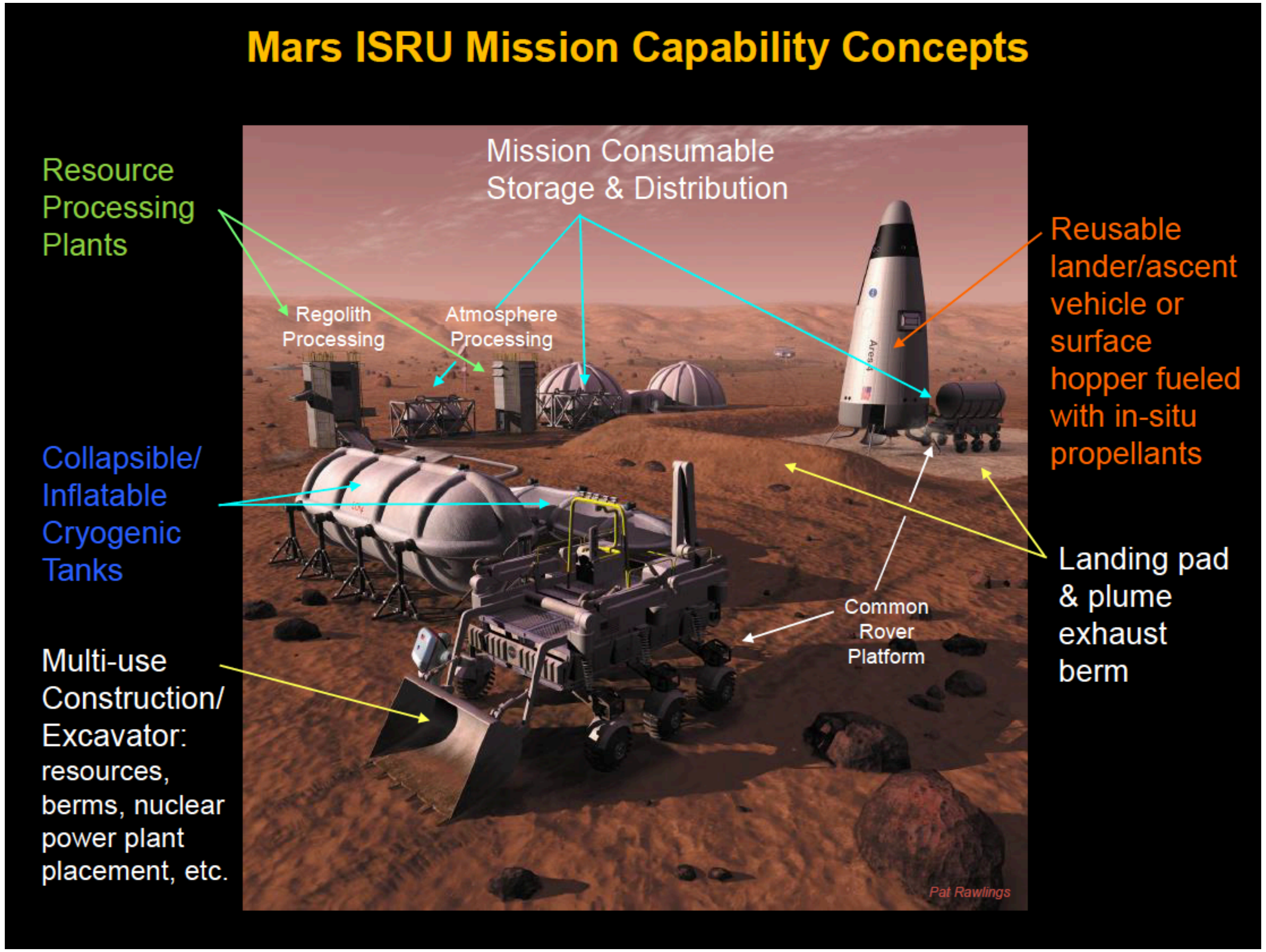
- Motivation
- Technology Overview
- Geometries
- Modeling
- Technical Challenges
- System Challenges
- Life-Limiting Challenges
- Performance Challenges

Motivation

- In-Situ Resource Utilization (ISRU) is needed for long-term planetary (Lunar & Mars) exploration affordability and sustainability. ISRU can:
  1) Significantly reduce launch costs and mission risks
  2) Enhance and enable reusability of landers, space transportation and surface assets
  3) Support future space commercialization

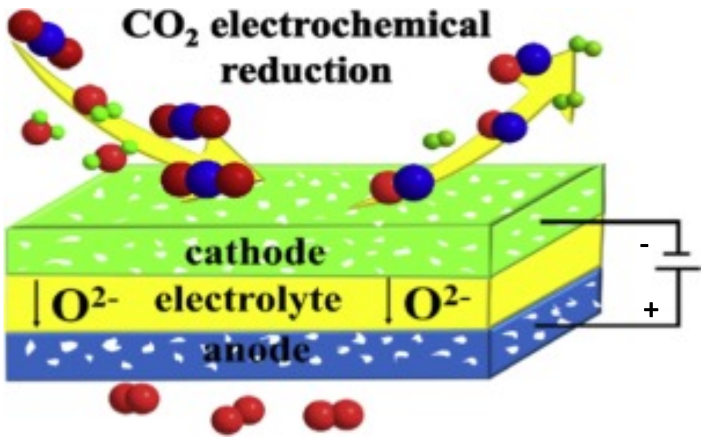
- ISRU is disruptive & game changing to lunar & Mars exploration architectures

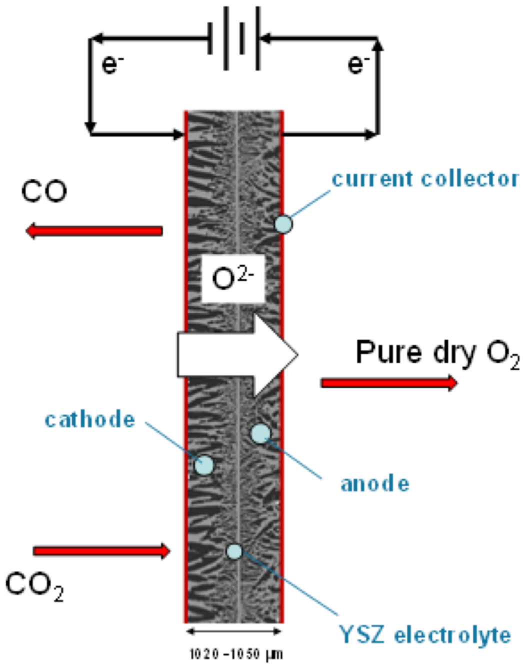
- ISRU can strongly influence architectures, design decisions, and technologies needed in other exploration elements based on:
  1) ISRU capabilities needed from other elements
  2) ISRU product availability (ex. degree of life support closure required)



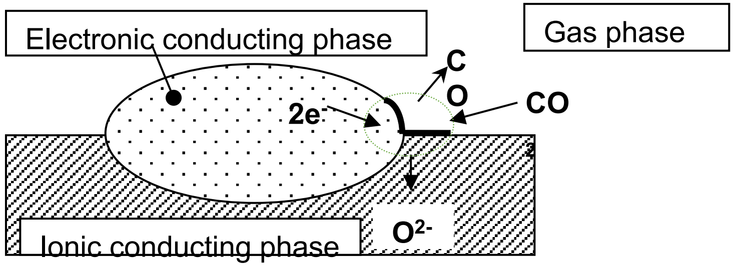
Solid Oxide Electrolysis (SOE) Overview

- What is SOE?
  - SOE is the process in which oxygen is generated by conducting oxygen ions across a solid, non-porous electrolyte.
  - SOE works on the principle that at elevated temperatures (800-1000 deg C), the ceramic electrolyte (yttria-stabilized zirconia) becomes conductive to oxygen ions.
  - A thin membrane of YSZ is sandwiched between cathode & anode electrodes.
  - The electrodes are porous, which creates many Three-Phase Boundaries, referring to an interface between the electrolyte phase, electrode phase and gas phase.
  - For oxygen separation process to begin, the CO_2 must diffuse through the porous electrode and come into the vicinity of a three-phase boundary.
  - Through a combination of thermal dissociation and Electrocatalysis, an oxygen atom is liberated from the CO_2 molecule and picks up two electrons from the cathode to an oxygen ion.



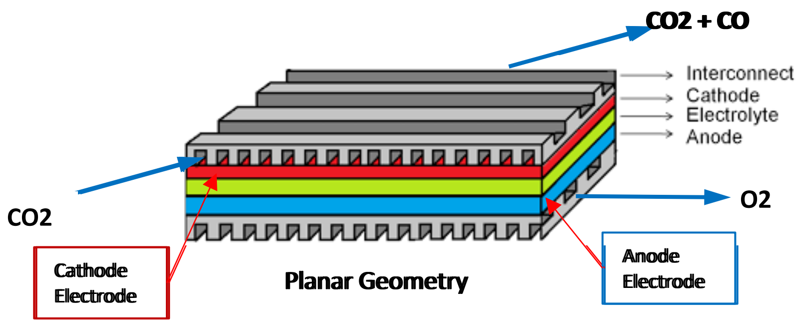


Triple-Phase Boundary (TPB)

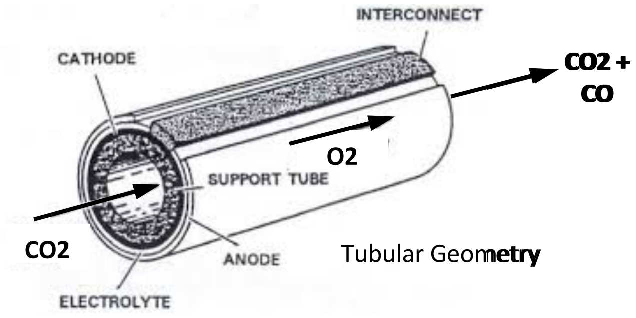


CO_2 reduction: $CO_2 + 2e^- \leftrightarrow CO + O^{2-}$

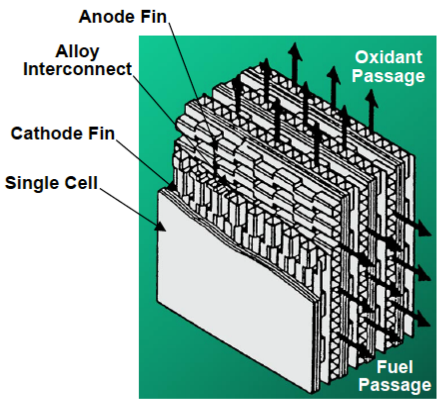
SOE Geometries



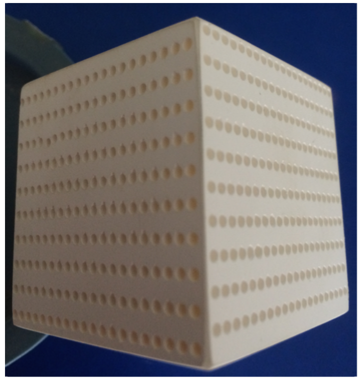
Planar Geometry



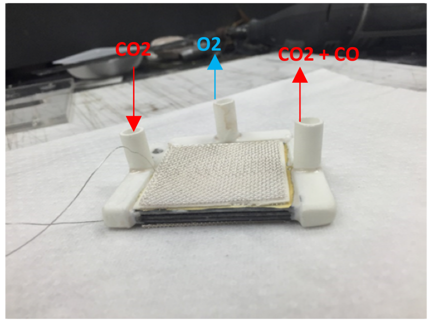
Tubular Geometry



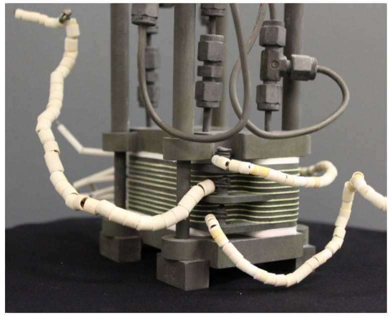
Monolithic


Honeycomb

- Planar stacks operated at higher efficiency than Tubular designs.
- Tubular system is able to operate at higher delta-P then Planer.
- Integration of external edge manifold to planar stack is very challenging.
- External leakage, thermal cycling /expansions, limited thermal ramp rate and crack/crack propagation are SOE technology limitations.
- SOE advancements are included in the ISRU SBIRs and BAA.

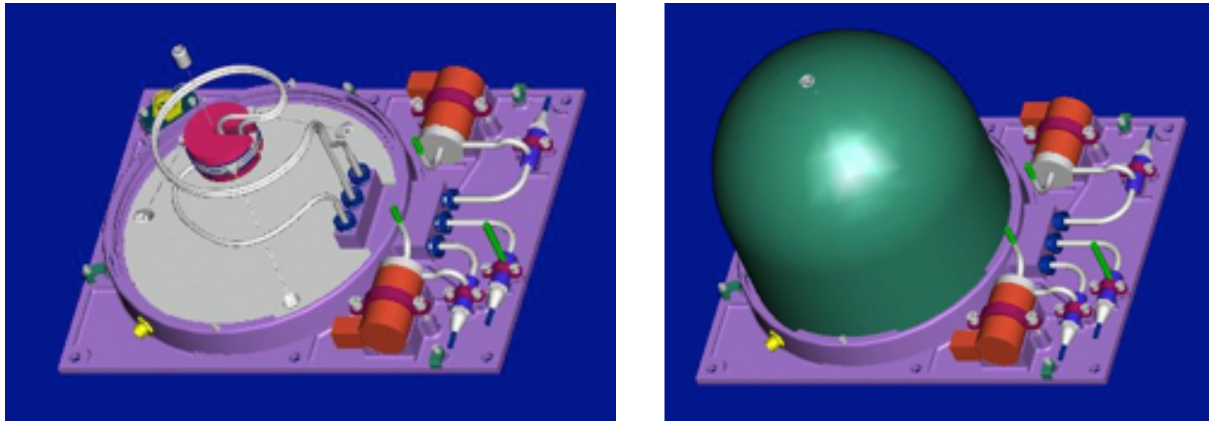


External Edge Manifold

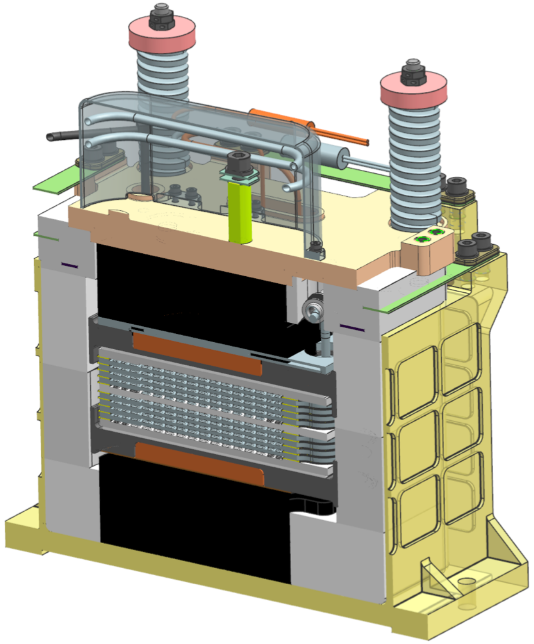

Internal Manifold

Modeling Objectives

- SOE stack sizing & 2-D heat transfer and thermal insulation design
- Create a geometry and mesh of a MOXIE stack.
- Initially, a single SOXE plate will be modeled and analyzed for both fluids and solid modeling.
- Initial solid model uses flat surfaces, ignoring flow channels.
- Heat transfer and reaction kinetics will then be added to the fluid flow model.
- Eventually, more cells will be added to the model and plate with flow channels will be modeled.
- Parametric analyses on the structural/thermal model will be performed.



2001 Mars ISPP Precursor (MIP) Single-Stack Assembly



Mars 2020 MOXIE SOXE Assembly

Solid Oxide CO_2 Electrolysis Cell-Stack Sizing Model

Solid Oxide CO2 Electrolysis Cell-Stack Design

INPUT VALUES

OPERATING CONDITIONS

Mission Duration					day,	1
Inlet CO2 Pressure	pa,	50662.5	psi,	7.35	atm,	0.5
Outlet O2 Pressure	pa,	75993.75	psi,	11.025	atm,	0.75
Operation Time					hour,	24
Operating Temperature			Degree C	850	K,	1123
Total O2 Production	g/hr,	1100	g/min,	18.333	scc/min,	14113.0
Number of Stack					#,	4
Cell Voltage					V,	1.2
Current Density					mA/cm^2,	400
Cell Resistance					Ohm,	0.01

Note: Typically 500 mA/cm^2 is the maximum Electrode/Electrolyte Current Density used in Solid Oxide Electrolysis.

Note: System power efficiency is based on Cell Resistance
Ideal Cell Resistance ≤ 0.005 Ohm
Typical Cell Resistance = 0.03 Ohm
Poor Cell Resistance > 0.03 Ohm

Key Factors:

1. Operating voltage
2. Current density (mA/cm^2)
3. Cell resistance
4. Operating temperature
5. Electrolyte density
6. Electrode materials & density
7. Utilization efficiency

CELL DIMENSIONS, RECTANGULAR

	Electrolyte Information		
1	Length YSZ L_1	cm,	12
2	Width YSZ W_1	cm,	12
3	Electrolyte Thickness T_1	cm,	0.04
4	Zirconia Density	kg/cm^3,	0.05333

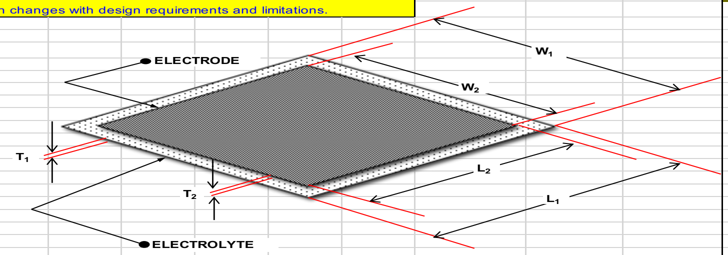
Note: Typical electrolyte thickness ranges are,
cm, 0.02 to 0.05
in, 7.874E-3 to 1.97E-2

	Electrode Information		
1	Length L_2	cm,	10
2	Width W_2	cm,	10
3	Electrode Thickness T_2	cm,	0.005
4	Electrode Ink Density	kg/cm^3,	0.02145

Note: Electrode Ink or paste can be made of several materials, such as Platinum, Conductive Ceramics or any other conductive materials.

	Distribution Plate Information		
1	Distribution Plate Length	cm,	12
2	Distribution Plate Width	cm,	12
3	Distribution Plate Thickness	cm,	0.2
4	Distribution Plate Density	kg/cm^3,	0.0072

Note: Distribution plat thickness is function of the design, which changes with design requirements and limitations.



CELL DIMENSIONS, CIRCULAR

	Electrolyte Information		
1	Radius YSZ R_1	cm,	6.6
2	Electrolyte Thickness T_1	cm,	0.04
3	Zirconia Density	kg/cm^3,	0.05333

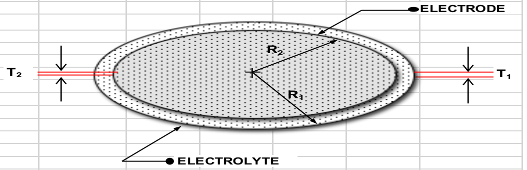
Note: Typical electrolyte thickness ranges are,
cm, 0.005 to 0.5
in, 1.97E-3 to 1.97E-2

	Electrode Information		
1	Radius R_2	cm,	5.6
2	Electrode Thickness T_2	cm,	0.005
3	Electrode Ink Density	kg/cm^3,	0.02145

Note: Electrode Ink or paste can be made of several materials, such as Platinum, Conductive Ceramics or any other conductive materials.

	Distribution Plate Information		
1	Distribution Plate Radius	cm,	6.6
2	Distribution Plate Thickness	cm,	0.2
3	Distribution Plate Density	kg/cm^3,	0.0072

Note: Distribution plat thickness is function of the design, which changes with design requirements and limitations.



OUTPUT VALUES, RECTANGULAR

	Electrolyte Information		
1	Area YSZ	cm^2,	144
2	Electrolyte Volume	cm^3,	5.76
3	Total Volume, Vx(#cell)	cm^3,	531.17
	Electrode Information		
1	Area Platinum	cm^2,	100
2	Electrode Volume	cm^3,	0.5
3	Total Volume, V x (#cell x 2)	cm^3,	92.22
	Distribution Plate Information		
1	Distribution Plate Area	cm^2,	144
2	Distribution Plate Volume	cm^3,	28.8
3	Total Volume, Vx(#cell + 1)	cm^3,	2684.63

CELL PERFORMANCE

Current	A,	40
Ohmic Cell Power	W,	16.0
Cell Power	W,	48
Total Cell Power	W,	64.0
O2 Production [Current x (1/5.33399) x(Tk-amb/Ppsi-amb)]	scc/min,	153.0
O2 Production	g/min,	0.199
O2 Production	g/hour,	11.9
Total O2 Production per cell	g/operation,	286.3
Chemical Conversion Efficiency η_{ch}	%,	$30 \le \eta \le 40$

Note: The chemical conversion efficiency is the same as CO2 to O2 conversion factor. This value has been evaluated only experimentally.
$X * CO_2 \text{------>} (X * \eta) * CO + (X * \eta)/2 * O_2$

STACK PERFORMANCE

Total Number Of Cells	#,	92
Number Of Cells Per Stack	# / stack,	23
Stack's Nenst Voltage	V,	27.3556479
Total Nernst & Free Energy Power	W,	1094.22591
Total Ohmic Power	W,	1475.5
Stacks Power	W,	4426.38258

Total Stacks Current	A,	3688.7
Total Voltage	V,	174.9
Total Power (Ohmic power + Nerrst & Free Energy Power+ Stacks pov	W,	6996.1
Total O2 Production	scc/min,	14113.0027
Total O2 Production Per Operation	g/operation,	26400
Stack Weight	gram,	12564
Stack Height	cm,	23.2540759
Weight	gram,	50256.53
Total Height	cm,	93.02

OUTPUT VALUES, CIRCULAR

	Electrolyte Information		
1	Area YSZ	cm^2,	136.847776
2	Electrolyte Volume	cm^3,	5.47391104
3	Total Volume, Vx(#cell)	cm^3,	512.37
	Electrode Information		
1	Area Pt	cm^2,	98.52034562
2	Electrode Volume	cm^3,	0.492601728
3	Total Volume, V x (#cell x 2)	cm^3,	92.22
	Distribution Plate Information		
1	Distribution Plate Area	cm^2,	136.847776
2	Distribution Plate Volume	cm^3,	27.3695552
3	Total Volume, Vx(#cell + 1)	cm^3,	2589.19

CELL PERFORMANCE

Current	A,	39.40813825
Ohmic Cell Power	W,	15.5300136
Cell Power	W,	47.2897659
Total Cell Power	W,	62.8197795
O2 Production	scc/min,	150.8
O2 Production	g/min,	0.196
O2 Production	g/hour,	11.75197614
O2 Production Per Cell Per Operation	g/operation,	282.0474273
Chemical Conversion Efficiency η_{ch}	%,	$30 \le \eta \le 40$

Note: The chemical conversion efficiency is the same as CO2 to O2 conversion factor. This value has been evaluated only experimentally.
$X * CO_2 \text{------>} (X * \eta) * CO + (X * \eta)/2 * O_2$

STAKS PERFORMANCE

Total Number Of Cells	#,	94
Number Of Cells Per Stack	# / stack,	23
Nernst Staks Voltage	V,	27.7665
Total Nernst & Free Energy Power	W,	1094.225915
Total Ohmic Power	W,	1453.629139
Total Cell Power	W,	4426.382582

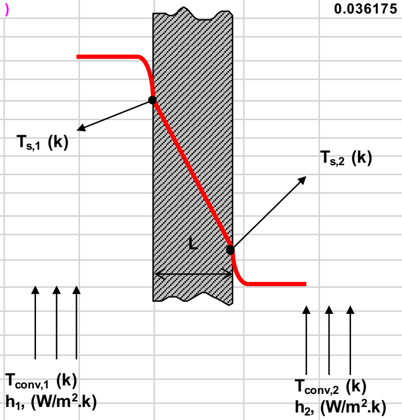
Total Staks Current	A,	3688.652152
Total Voltage	V,	177.0
Total Power	W,	6974.237637
Total O2 Production	scc/min,	14113.00271
Total O2 Production Per Operation	g/operation,	26400
Stack Weight	gram,	12134
Stack Height	cm,	23.60031981
Weight	gram,	48535.85512
Total Height	cm,	94.40127923

Thermal Insulation Design Model

Constants

$K(T) = a * T_i^2 + b * T_i + c$

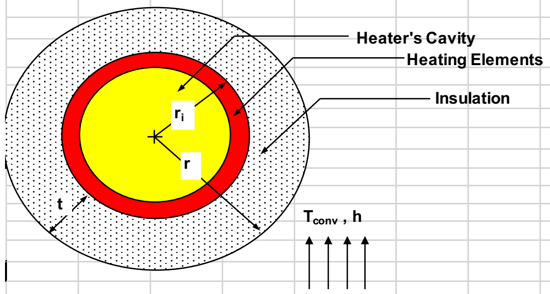
	MIN-K TE-1400
a, ($W/m.k^3$)	5.6849E-08
b, ($W/m.k^2$)	-3.511E-05
c, (W/m.k)	0.036175



OUTPUT VALUES

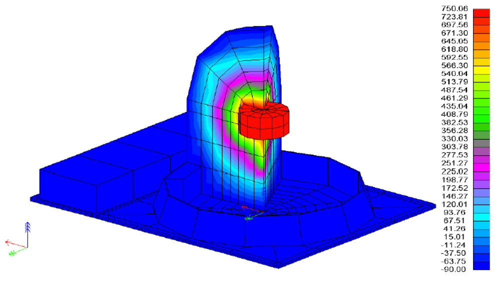
K, Thermal Conductivity (W/m.k)					0.05241072			
K, Thermal Conductivity (W/m.k)					0.03			
A, Surface Area		Heater #1	m^2,	0.0126	cm^2,	126	in^2,	19.52996
		Heater #2	m^2,	0.0126	cm^2,	126	in^2,	19.52996
L, Insulation Thickness			m,	0.127682	cm,	12.768	in,	5.026854
Insulation Volume			m^3,	0.046024	cm^3,	4.60E+04	in^3,	2808.546
Total Weight			kg,	4.423809	lb,	9.754		
	0.0381							
r	0.019489		-0.0186112	-1.86112	-0.7327246			

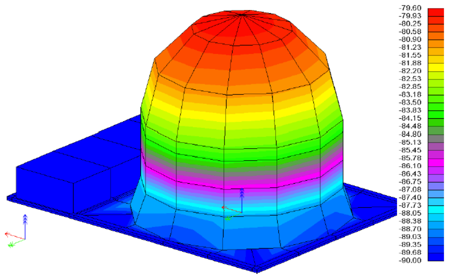
Insulation Calculation for Cylindrical Heater



ri, Initial Heater Radius	in,	3.5433	cm,	9
h, Heater's height	in,	5.622036	cm,	14.28
h, Convection Coefficient			W/m^2.k,	2.68928
K, Thermal Conductivity of Insulation			W/m.k,	0.05241
r, Insulation Plus Heater Radial Thickness	in,	4.31057	cm,	10.94888
t, Insulation Radial Thickness	in,	0.76727	cm,	1.94888
V, Insulation Volume	in^3,	67.0829	cm^3,	170.3909

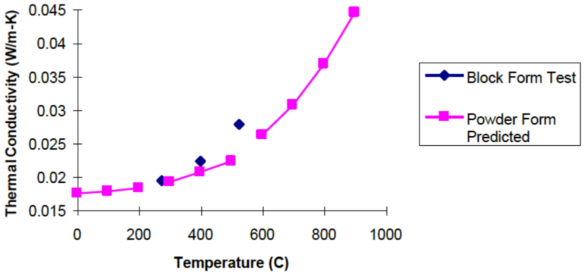
- **THERMAL ANALYSIS: (continued)**
  - Steady State Cold Day (Worst Case)
    * 9.515W heater power and -90°C MIP box environment



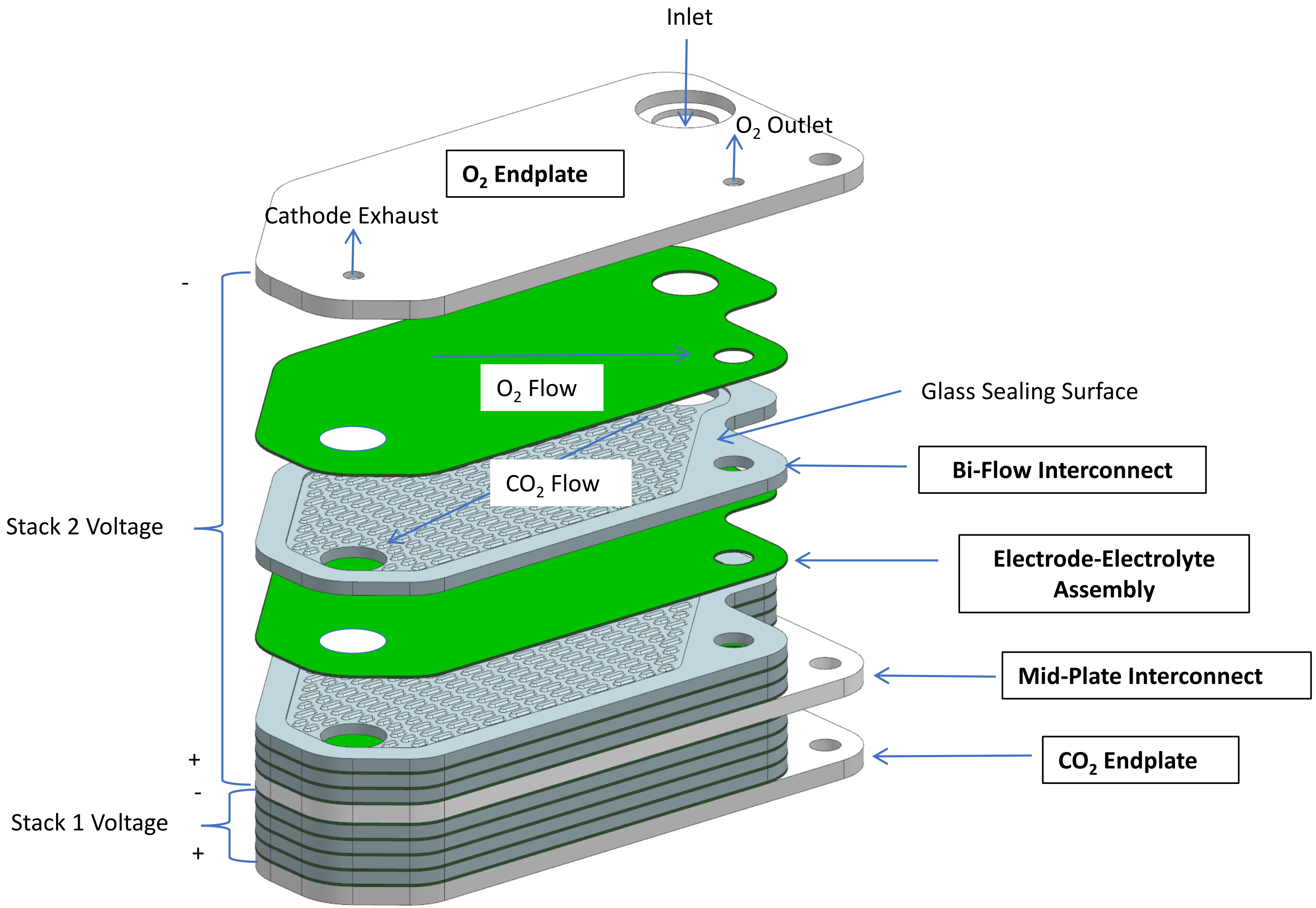


- **THERMAL INSULATION: OG Dome**
  - Thermal Ceramics (Min-K) TE-1400:
    * "Crushed" form of the insulation is used to fill OG dome.
      - Promotes much easier assembly than the block form (reduced fabrication effort)
      - Lower thermal losses than the block form (no gaps between blocks)
    * Insulation performance:
      - External surface temperature maintained < 15°C above ambient during OGS operations
      - Demonstrated multiple full thermal cycle operations with no noticeable degradation
    * Insulation characteristics:
      - Major contents are silica and fibrous glass. (MSDS available upon request)
      - Density: 0.333195 g/cm^3 (20.8 Lbm/ft^3) block form
      - Thermal conductivity (see graph below)

TE-1400 Insulation Thermal Conductivity

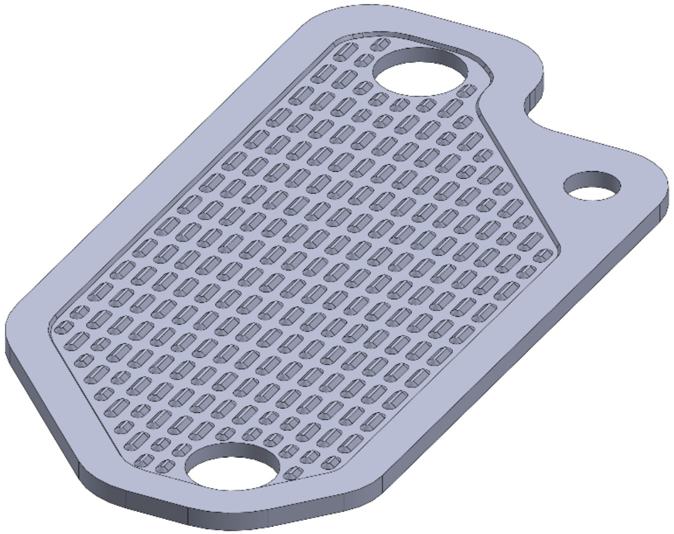


SOXE Stack Construction
(Tubes and Bus Bars not Shown)

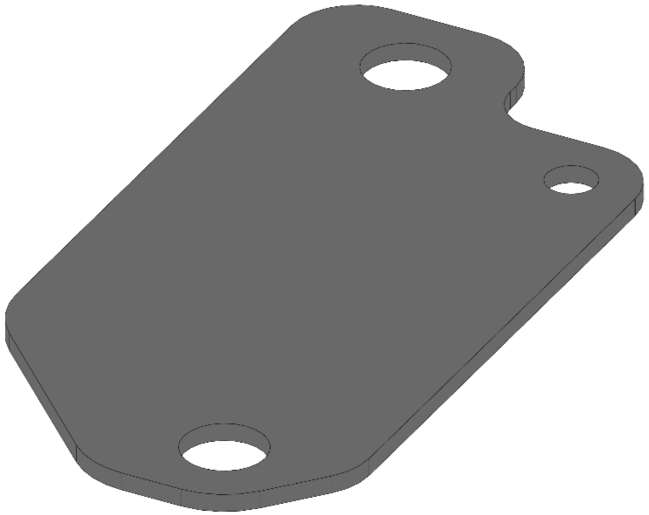


Solid geometry developed from SOXE drawings

- Fully detailed solid geometry built from flat drawings for fluids and advanced mechanical models

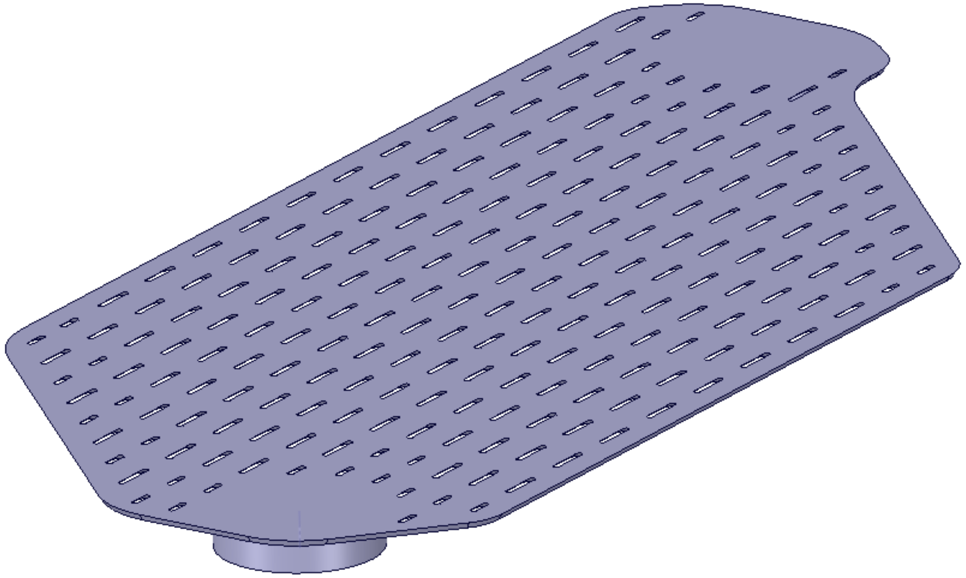


Flat-top solid geometry developed for initial mechanical models

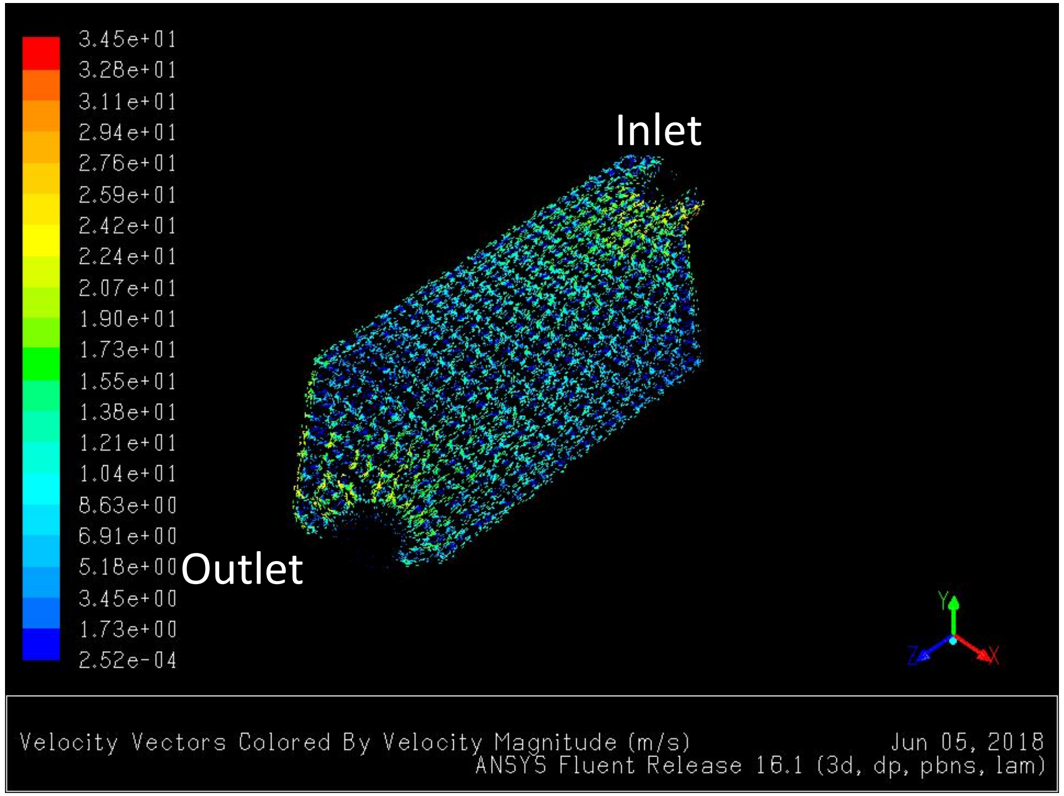


Flow-only model

- Fluid volume extracted from voids in solid geometry

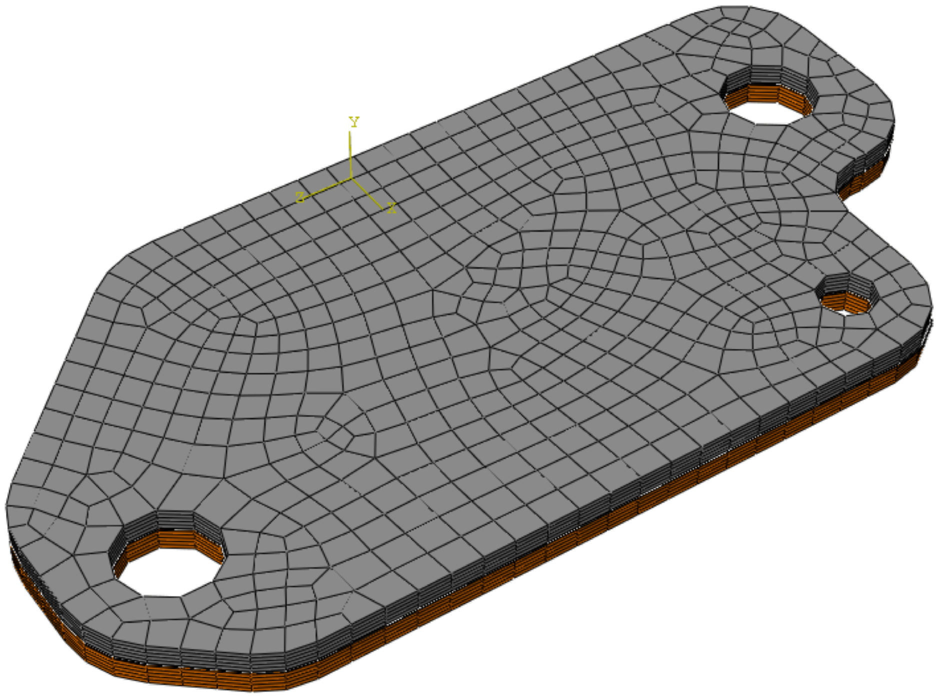


- Initial fluid models developed to examine flow through CO_2 channels

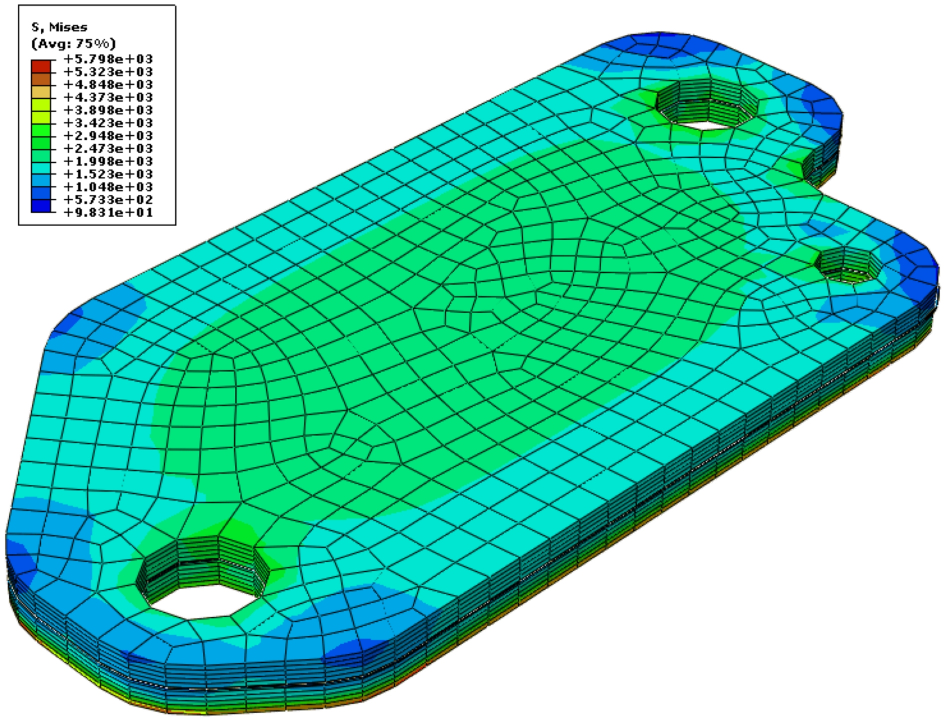


Solid model

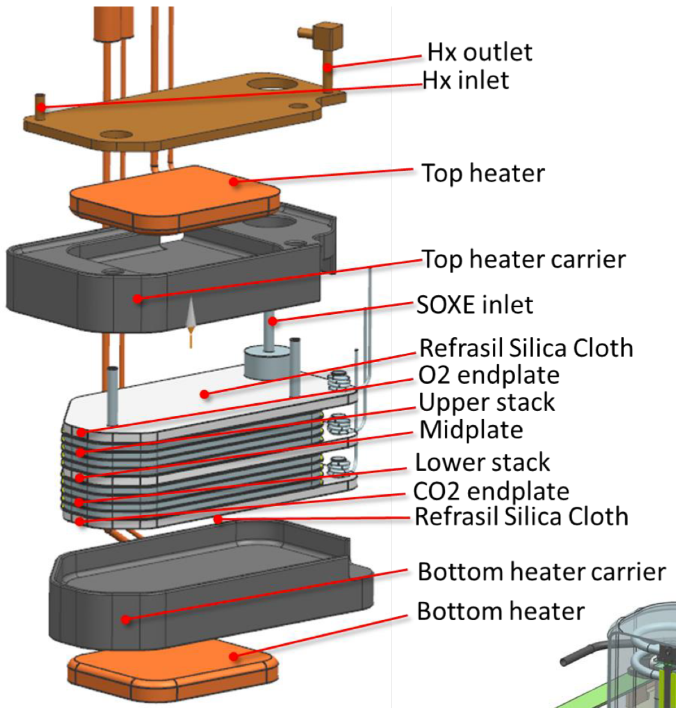
- Single cell with electrolyte layer

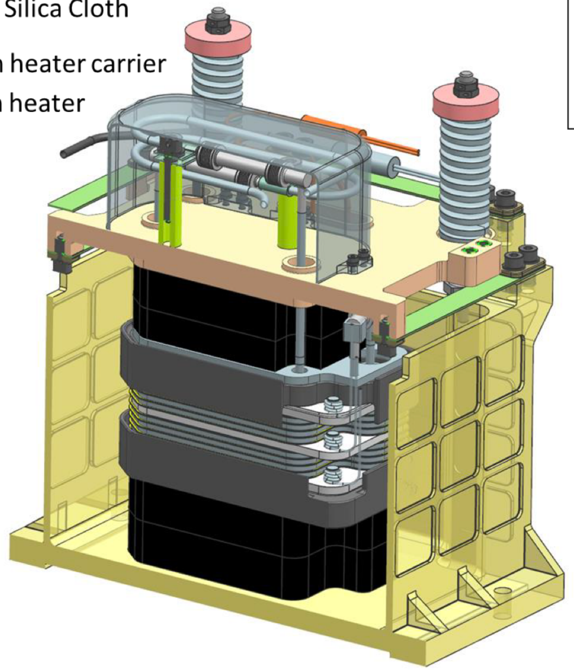


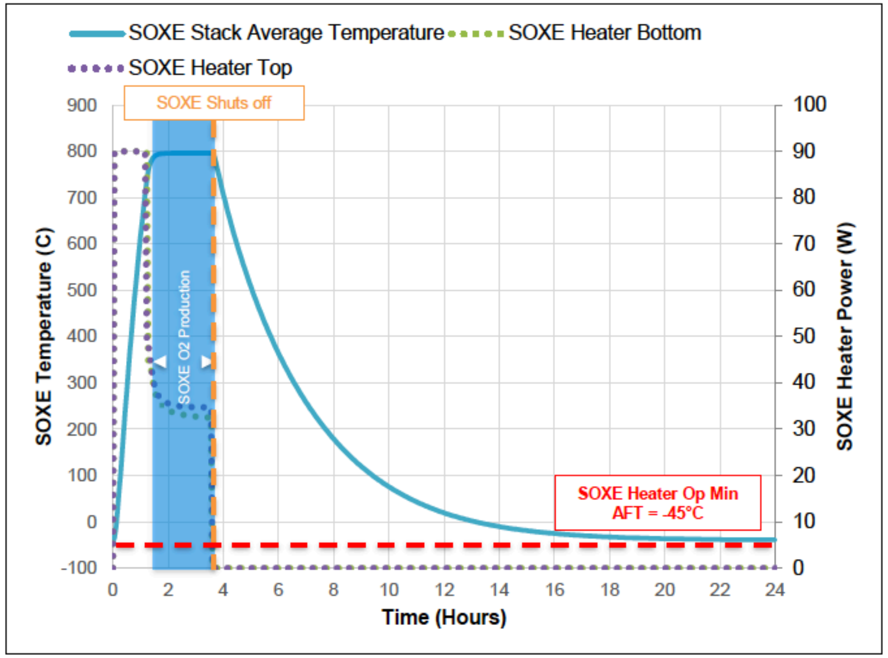
- Stress distribution

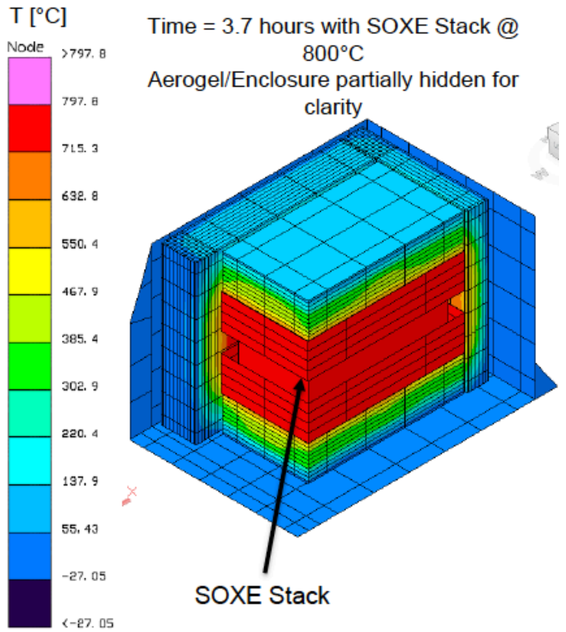


Thermal Analysis of MOXIE SOXE Stack





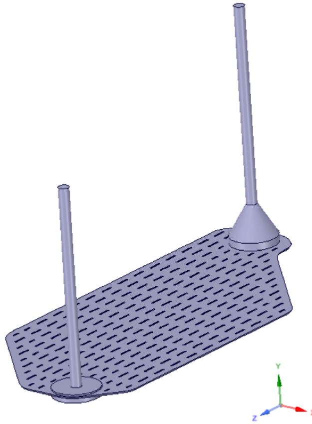




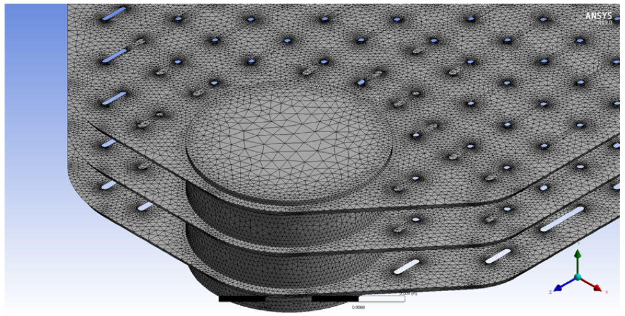
- WCC Operation assumes SOXE is warmed up to 800°C and operates for 2 hours; Electronics power is turned on, but no gas flowing (no Motor/Compressor Power dissipation)
- SOXE Warm-up time takes ~85 minutes; matched with SOXE warm-up time in testing (July 2016)
- SOXE Heat Leak during O2 production ~70 W
- SOXE Min Op AFT of -45°C, SOXE average temperatures drops to -36°C after SOXE shuts off

NASA Internal Future Modeling Directions

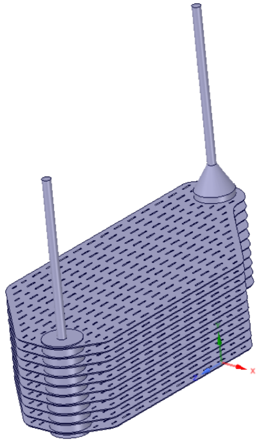
- Incremental approach to models
  - Initial fluids model is fluid flow only.
  - Thermal physics to be added to flow model.
  - Chemistry to be added to thermal/flow model
  - Initial solid model eliminates gas channels
  - Obtain actual thermal and mechanical properties for various cell materials.
  - Obtain the value of the clamping force
  - Increase number of layers and model the flow channels for realistic geometry for solid modeling



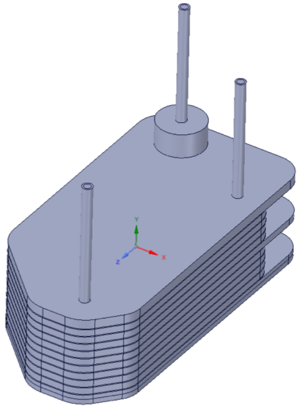
Grid for single-stack fluid model



Grid for 3-stack fluid model



Grid for 10-stack fluid model



10-stack fluid model

Solid Oxide CO_2 Electrolysis Technology Challenges

- **High temperature operation (800-1000 deg C)**
  - Limits available material
  - Complicated design to compensate for dimensional changes
- **Thermal cycling**
  - CTE mis-match, thermal gradients due to poor thermal conductivity of ceramic layers.
  - Effects CONOPS (i.e. start-up time).
- **Performance degradation**
  - CO_2 reduction cathode degrades without CO in dry CO_2.
  - Anode (delamination of electrode layer under high current density, high ionic O^{2-} flux).
  - Carbon deposition (coking) at high CO/CO_2 gas ratios. (Limits CO_2 utilization/conversion).
- **Structural integrity**
  - Maintain stable in-plane (x/y) support/alignment.
  - Close tolerances on metal-to-ceramic interfaces.
- **Sealing**
  - Sealing for long-term high temperature operation.
  - Thermal cycling over large ΔT adds additional challenges.
- **Packaging**
  - High temperature thermal insulation, external connection isolation (electrical heaters, gas connections, etc.

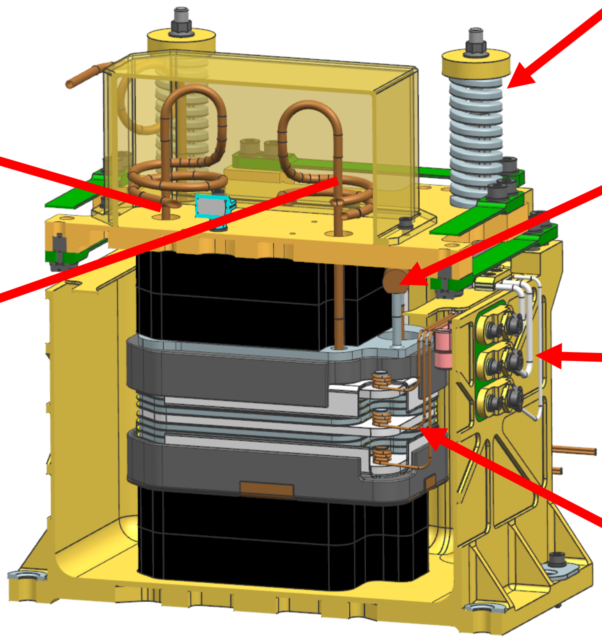
Mars 2020 SOXE Systems Challenges

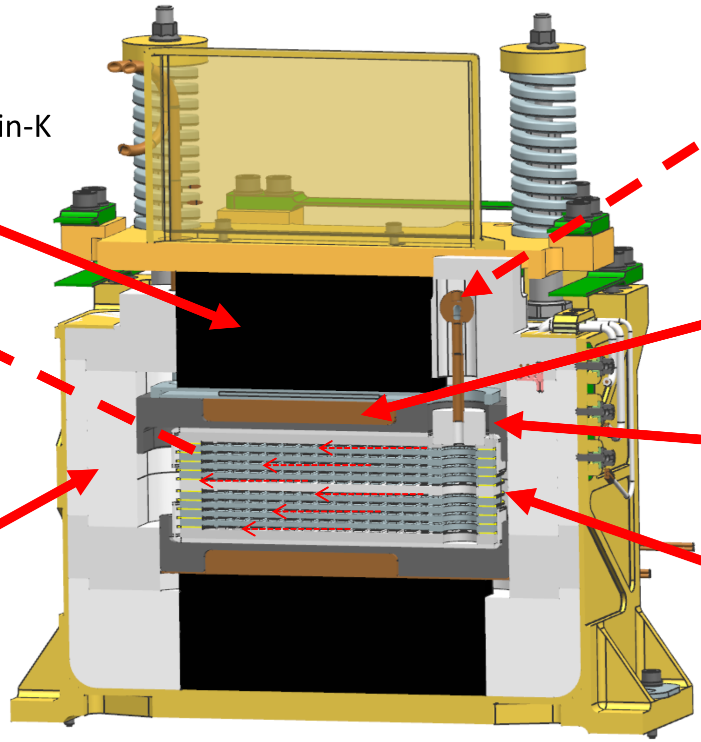
- **Packaging**
  - Insulation
    - Uniform insulation around stack capable of withstanding launch/landing vibration
  - Compression
    - Maintaining uniform compression to ensure sealing and electrical conductivity throughout stack
  - Accommodating instrumentation
    - Incorporation of adequate connections for monitoring stack ‘health’ and conditions during range of operations
- **Controls**
  - Stack Operational Information
    - Coordination of stack operating limits and fault tolerance with response
  - Integration with instrumentation
    - Algorithms of software integral with stack operational limits/ranges and monitors
- **Instrumentation**
  - Thermal and electrical information at appropriate critical locations within stack and supporting infrastructure

SOXE Life-limiting Challenges

- **Non-uniformity in design**
  - Cell-to-cell performance differential
    - Uniformity of cell-to-cell chemistry
    - Uniformity of feedstock to cells throughout stack
  - Thermal
    - Choice of insulation materials
    - Breakdown of insulation materials (thermal/mechanical) over time
  - Compression
    - Three dimensional sealing and conductivity mismatch over surface and length of stack
- **Non-uniformity in operations**
  - Heatup ramp rate not commensurate with materials
  - Startup conditions inadequate for conversion/catalyst
- **Operational constraints**
  - Inadequate information for control of operating limits
- **Feedstock**
  - Maintaining proper feedstock composition at stack inlet

MOXIE SOXE Stack Assembly (Internal)





(Red arrows in stack show the flow of CO/CO_2 through the stack)

- SOE for manned mission is significantly different design
  - MOXIE produces 20 gm of O_2/hr
  - Manned Mission requires 2.2. kg of O_2/hr

SOXE Performance Issues

- **Operating temperature**
  - High temperature pushes limit of seals and ion migration across interfaces
  - Alteration of kinetics of catalysts and transport
  - Carbon deposition on cathode
- **Operational limits**
  - Changes in performance with time
  - Control response and monitor accuracy
- **Control of operating limits**
  - Instrumentation adequate to sense stack 'health'
  - Ability to compensate operations with limits
- **Design of stack**
  - Internal or external manifolds for maintaining flow uniformity over operations
  - Flow field and electrical conductivity designs
- **TOT**
  - Degradation of electrodes to manage performance at limits
  - Understanding 'sweet spot' of operations for long term operation
- **Materials selection mismatch**
  - Wide range of cathode, anode, electrolyte compositions most appropriate for feedstock and operating conditions
  - Wide range of interface materials commensurate with selected cathode, anode and electrolyte choices for control of ion migration

Summary

- **Benefits**
  - Solid Oxide Electrolysis has higher utilization efficiency compare to lower-temp technologies
  - SOE generates dry-O_2 from various feedstocks (dry-CO_2, CO_2 + H_2O, and H_2O)

- **Challenges and limitations**
  - High temperature (800-1000 deg C) operation limits the used of various materials
  - External Leakage, thermal Cycle, thermal expansion, fast ramp-up and ramp-down rates, and structural integrity are SOE technology limitations.
  - Sealing for long-term high temperature operation. Limited work in other technologies above 700 deg C

- **Design Phase Implementation**
  - Parametric analyses on the structural/thermal model
  - Thermal management and thermal integration

Thank You for Your Attention

Questions