







NASA Johnson Space Center Thermal and Fluids Analysis Workshop

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Solid Oxide CO₂ Electrolysis Technical Overview

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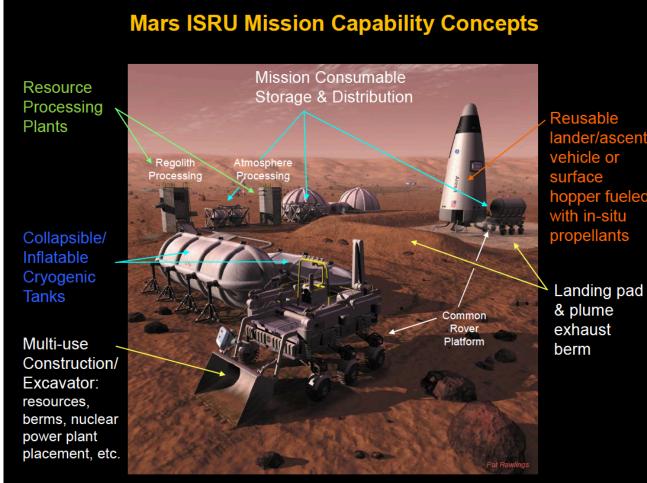


- Motivation
- Technology Overview
- Geometries
- Modeling
- Technical Challenges
- System Challenges
- Life-Limiting Challenges
- Performance Challenges



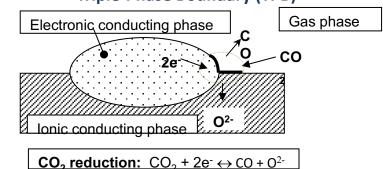
Motivation

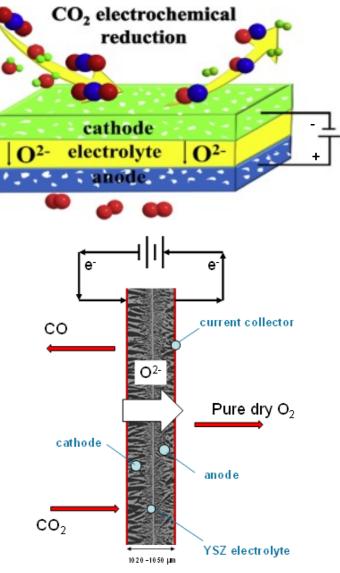
- In-Situ Resource Utilization (ISRU) is needed for long-term planetary (Lunar & Mars) exploration affordability and sustainability. ISRU can:
 - 1) Significantly reduce launch costs and mission risks
 - 2) Enhance and enable reusability of landers, space transportation and surface assets
 - 3) Support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





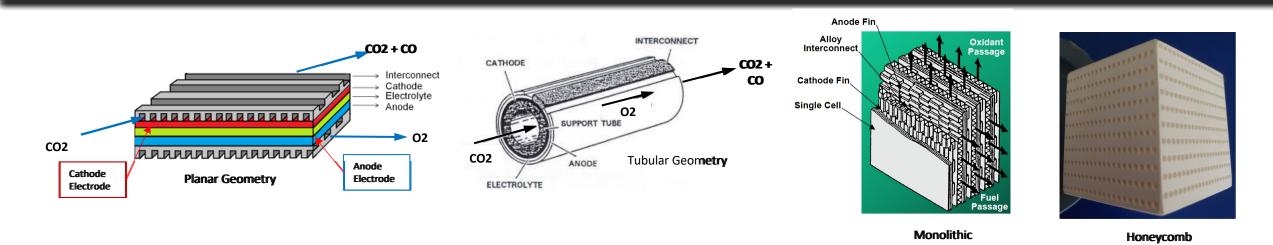
- What is SOE?
 - SOE is the process in which oxygen is generated by conducting oxygen ions across a solid, non-porous electrolyte.
 - SOE works on the principle that at elevated temperatures (800-1000 deg C), the ceramic electrolyte (yttria-stabilized zirconia) becomes conductive to oxygen ions.
 - 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 CO₂ 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 CO₂ molecule and picks up two electrons from the cathode to an oxygen ion.
 Triple-Phase Boundary (TPB)



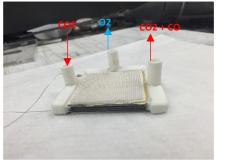




SOE Geometries



- 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.



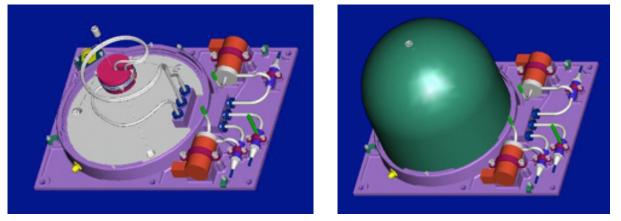
External Edge Manifold



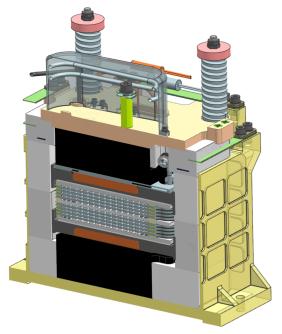
Internal Manifold



- 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



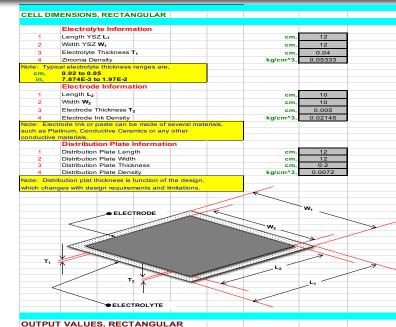
Mars 2020 MOXIE SOXE Assembly



Solid Oxide CO₂ Electrolysis Cell-Stack Sizing Model

Solid Oxide CO2 Electrolysis Cell-Stack Design

INPUT VALUES						
OPERATING COND	ITIONS					
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	К,	1123
Total O2 Production	g/hr,	1100	g/min,	18.333	scc/min,	14113.0
Number of Stack					#,	4
Cell Voltage					۷.	1.2
Current Density					mA/cm^2,	400
Note: Typically 500 mA Current Density used in				ctrolyte		
Cell Resistance					Ohm,	0.01
Note: System power ef	ficiency is b	ased on Ce	Il Resistance			
Ideal Cell Resistance ≤	0.005 Ohi	m				
Typical Cell Resistance	= 0.03 Ohn	n				
Poor Cell Resistance >	0.03 Ohm					



Key Factors:

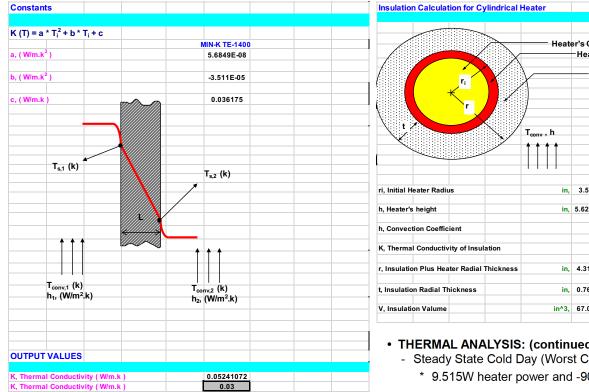
- 1. Operating voltage
- 2. Current density (mA/cm²)
- 3. Cell resistance
- 4. Operating temperature
- 5. Electrolyte density
- 6. Electrode materials & density
- 7. Utilization efficiency

	Electrolyte Inform	ation					
1	Area YSZ				cm^2.	144	
2	Electrolyte Volume				cm^3.	5.76	
3	Total Volume, Vx(#cell)			cm^3,	531.17	
	Electrode Informat	tion					
1	Area Platinum				cm^2.	100	
2	Electrode Volume				cm^3,	0.5	
3	Total Volume, V x (#ce	II x 2)			cm^3,	92.22	
	Distribution Plate I	nformatio	on				
1	Distribution Plate Area				cm^2,	144	
2	Distribution Plate Volu	me			cm^3,	28.8	
3	Total Volume, Vx(#cell	+ 1)			cm^3,	2684.63	
CELL PE	RFORMANCE						
Current					А,	40	
Ohmic Cell F	ower				W,	16.0	
Cell Power					W,	48	
Total Cell Po	ower				w.	64.0	
O2 Producti	on [Current x (1/5.3339	9) x(Tk-amb	/Ppsi-amb)]		scc/min,	153.0	
O2 Producti	on				g/min,	0.199	
O2 Producti	on				g/hour,	11.9	
Total O2 Pro	duction per cell				g/operation.	286.3	
Chemical Conversion Efficiency n _{ch}							
	and the second					30 ≤η ≤40	
Chemical Co Note: The cl	nversion Efficiency n _{ch}	iency is the	same as		%,		
Chemical Co Note: The cl	nversion Efficiency n _{ch}	iency is the	same as been evalua	ted only ex	%,		
Chemical Co Note: The cl CO2 to O2 c	nversion Efficiency n _{ch}	iency is the value has t	een evalua	ted only ex	%,		
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Chemical Co Note: The cl CO2 to O2 c X * CO2	nversion Efficiency ¶ _{ch} nemical conversion effic conversion factor. This -> (<i>X</i> * ¶) ● CO + (<i>X</i> PERFORMANCE	iency is the value has t	een evalua	ted only ex	%,		
Chemical Co Note: The cl CO2 to O2 co X * CO2 STACK F Total Numbe	nversion Efficiency ¶ _{ch} nemical conversion effic conversion factor. This -> (<i>X</i> * ¶) ● CO + (<i>X</i> PERFORMANCE	iency is the value has t	een evalua	ted only ex	%,	30 ≤η≤40	
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Chemical Co Note: The cl CO2 to O2 co X * CO2	nversion Efficiency η_{ch} nemical conversion efficiency ($x \cdot \eta$) $* CO + (x)$ PERFORMANCE or Of Cells Cells Per Stack st Voltage	iency is the value has t	een evalua	ted only ex	%, perimentally. #, # / stack, V,	30 ≤η≤40 92	
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Chemical Co Note: The cl CO2 to O2 co X * CO2 STACK I Total Number Number Of C Stack's Nens Total Nemst	nversion Efficiency η _{ch} nemical conversion effic conversion factor. This -> (X*η) * CO + (X PERFORMANCE or Of Cells Cells Per Stack st Voltage & Free Energy Power Power	iency is the value has t	een evalua	led only ex	, %, perimentally. #, # / stack, V, W,	30 ≤ ¶ ≤ 40 92 23 27.3556479 1094.22591	
Chemical Co Note: The d CO2 to O2 of CO2 to O2 of CO2 to O2 of CO2 STACK P Number Of C Stack's Nems Total Number Stacks Power	Inversion Efficiency ¶ _{ch} Isimical conversion efficiency conversion efficiency ⇒ (x * ŋ) * CC + (x PERFORMANCE PERFORMANCE Colls Per Stack at Voltage & Free Energy Power Power Power	iency is the value has t	een evalua	ted only ex	, %, perimentally. # / stack, V, W, W, W,	30 ≤ ¶ ≤ 40 92 23 27.3556479 1094.22591 1475.5	
Chemical Cc Note: The d CO2 to O2 co X * CO2 STACK I Total Number Number Of C Stack's Nen: Total Nemst Total Nemst Total Stacks Power Total Stacks	nversion Efficiency ¶ _{ch} nemical conversion effic conversion factor. This -> (X * ¶) ● CO + (X PERFORMANCE or Of Cells -> Colls Per Stack st Voltage & Free Energy Power Power ar Current	iency is the value has t	een evalua	ted only ex	, %, perimentally. # / stack, V, W, W, W,	30 ≤ ¶ ≤ 40 92 23 27.3556479 1094.22591 1475.5	
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Chemical Co Note: The cl CO2 to O2 c X * CO2 STACK IF Total Number Number O1 (Stack's Nem: Total Nemst Total Ohmic Stacks Power Total Obmic Total Voltag Total Power Total O2 Pro	Inversion Efficiency ¶ _{ct} Internation Efficiency ¶ _{ct} Internation Internation Internation (Conversion factor. This (Conversion factor. This (Conversion factor) (Conversion (Conversion)	iency is the value has t * ¶ y2 * O2	peen evalua		%, perimentally. # / stack, v, w, w, w, w, w, v, w, v, v, v, v, v,	30 ≤ η ≤ 40 92 23 27.3556479 1094.22591 1475.5 4426.38258 3688.7 174.9	
Chemical Co Note: The d CO2 to O2 c X * CO2	nversion Efficiency 1 _{tot} ismical conversion efficiency conversion factor. This ⇒ (X * 1) * CO + (X PERFORMANCE r Of Cells Zells Per Stack st Voltage & Free Energy Power Power of Comment (Ohmic power + Nerrst voluction Per Operation	iency is the value has t * ¶ y2 * O2	peen evalua		%, perimentally. # / stack, v, w, w, w, w, w, v, w, v, v, v, v, v,	30 ≤ η ≤ 40 92 23 27.3556479 1094.22591 1475.5 4426.38258 3688.7 174.9 6996.1 14113.0027	
Chemical Co Note: The cl CO2 to O2 c X * CO2 STACK IF Total Number Number O1 (Stack's Nem: Total Nemst Total Ohmic Stacks Power Total Obmic Total Voltag Total Power Total O2 Pro	nversion Efficiency 1 _{tot} ismical conversion efficiency conversion factor. This ⇒ (X * 1) * CO + (X PERFORMANCE r Of Cells Zells Per Stack st Voltage & Free Energy Power Power of Comment (Ohmic power + Nerrst voluction Per Operation	iency is the value has t * ¶ y2 * O2	peen evalua		%, perimentally. # / stack, V, W, W, W, V, V, V, V, V, V, V, V, V,	30 ≤ η ≤ 40 92 23 27.3556479 1094.22591 1475.5 4426.3258 3688.7 174.9 6996.1 14113.0027 26400	
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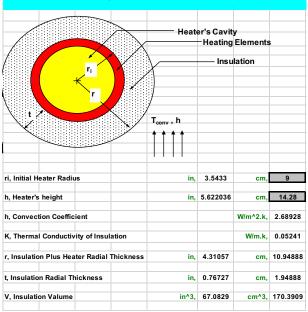
CELL DI	MENSIONS, C	CIRCULA	R				
	Electrolyte I	Informati	ion				
1	Radius YSZ R1					cm,	6.6
2	Electrolyte Thic	ckness T ₁				cm,	0.04
3	Zirconia Densit	ty				kg/cm^3,	0.05333
Note: Typi cm.	ical electrolyte th 0.005 to 0.5	hickness ra	anges are,				
in,	1.97E-3 to 1.9	7E-2					
1	Electrode In Radius R ₂	formatio	n			cm.	5.6
2	Electrode Thick	kness T ₂				cm, cm.	0.005
3	Electrode Ink E					kg/cm^3,	0.02145
Note: Elec	trode lnk or pas	ste can be			rials,	U	
such as Pla conductive	atinum, Conduc	tive Ceram	nics or any o	other			
conductive	materials.			1			
	Distribution						
1	Distribution Pla					cm,	6.6
2	Distribution Pla Distribution Pla	ate Thickne ate Density	ess			cm, kg/cm^3,	0.2
Note: Dist	ribution plat thic	kness is fu	unction of th	ne design,		ng/onr o,	0.0072
which char	nges with desigr	n requirem	ents and lin	nitations.			
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	Electrolyte I						
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1 2 3	Electrolyte I Area YSZ Electrolyte Volu Total Volume, Y Electrode In	Informati ume Vx(#cell)	ion			cm^3, cm^3,	5.47391104 512.37
1 2 3 1	Electrolyte I Area YSZ Electrolyte Volu Total Volume, Y Electrode In Area Pt	Informati ume Vx(#cell) iformatic	ion			cm^3, cm^3, cm^2.	5.47391104 512.37 98.52034562
1 2 3	Electrolyte I Area YSZ Electrolyte Volk Total Volume, Y Electrode In Area Pt Electrode Volume, Y Total Volume, Y	Informati ume Vx(#cell) iformatic ime V x (#cell >	ion on < 2)			cm^3, cm^3,	5.47391104 512.37
1 2 3 1 2 3	Electrolyte I Area YSZ Electrolyte Volu Total Volume, ' Electrode In Area Pt Electrode Volu Total Volume, ' Distribution	Information vx(#cell) information www. v x (#cell > Plate Inf	ion on < 2)			cm^3, cm^3, cm^2, cm^3, cm^3,	5.47391104 512.37 98.52034562 0.492601728 92.22
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1 2 3 1 2 3	Electrolyte I Area YSZ Electrolyte Vol. Total Volume, ' Electrode In Area Pt Electrode Volu Total Volume, ' Distribution Pla Distribution Pla	Information Vx(#cell) Iformation Ime V x (#cell > Plate Inf Plate Area ate Area	on (2) formation			cm^3, cm^3, cm^2, cm^3, cm^3, cm^3, cm^3,	5.47391104 512.37 98.52034562 0.492601728 92.22
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Thermal Insulation Design Model

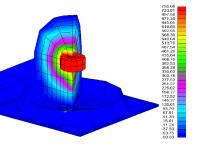


K, Therm	al Conductiv	vity (W/m.k)		0.03			
A, Surfac	e Area	Heater #1	m²,	0.0126	cm²,	126	in²,	19.52996
		Heater #2	m²,	0.0126	cm²,	126	in²,	19.52996
L, Insulat	ion Thickne	SS	m,	0.127682	cm,	12.768	in,	5.026854
Insulatior	1 Volume		m ³ ,	0.046024	cm³,	4.60E+04	in ³ ,	2808.546
Total Wei	ght		kg,	4.423809	lb,	9.754		
	0.0381							
r	0.019489		-0.0186112	-1.86112	-0.7327246			



• THERMAL ANALYSIS: (continued) - Steady State Cold Day (Worst Case)

* 9.515W heater power and -90°C MIP box environment

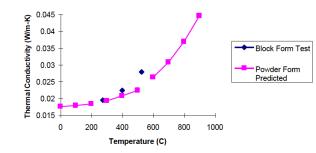


THERMAL INSULATION: OG Dome

- 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:

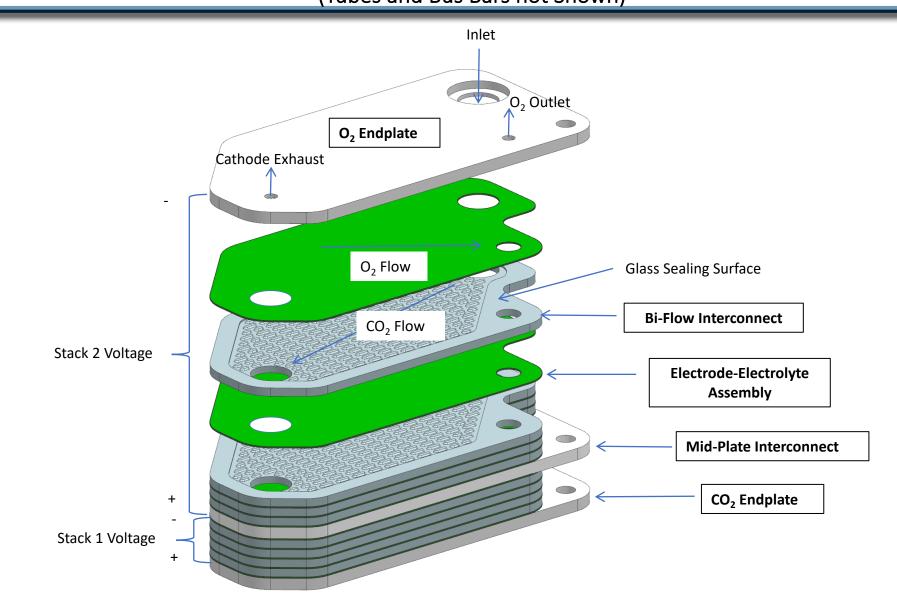
-79.93 -80.25 -80.90 -81.25 -81.55 -81.88 -82.25 -83.18 -83.25 -83.85 -83.85 -83.85 -84.45 -84.80 -85.45 -85.45 -85.45 -85.45 -86.43 -86.43

- Major contents are silica and fibrous glass. (MSDS available upon request)
- Density: 0.333195 g/cm³ (20.8 Lbm/ft³) block form
- Thermal conductivity (see graph below) TE-1400 Insulation Thermal Conductivity





SOXE Stack Construction (Tubes and Bus Bars not Shown)





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

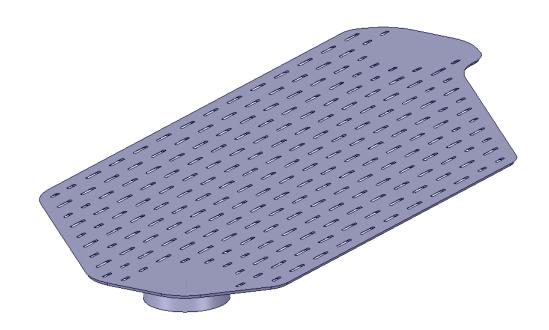
Flat-top solid geometry developed for initial mechanical models



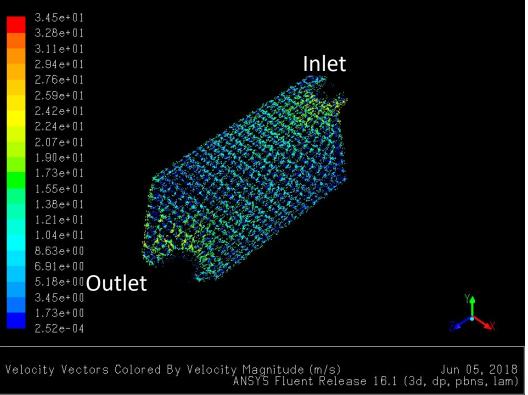




• Fluid volume extracted from voids in solid geometry



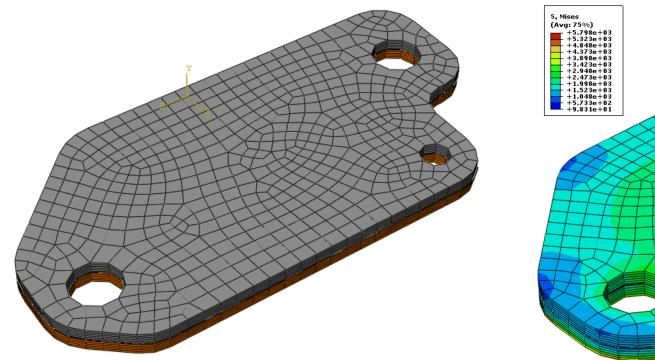
 Initial fluid models developed to examine flow through CO₂ channels

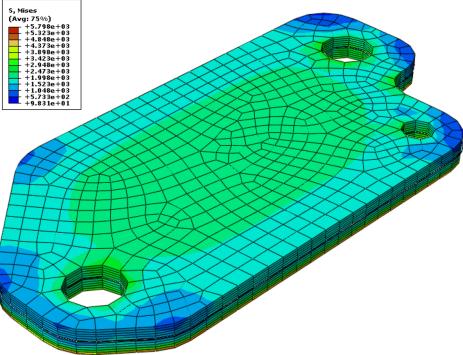




Solid model

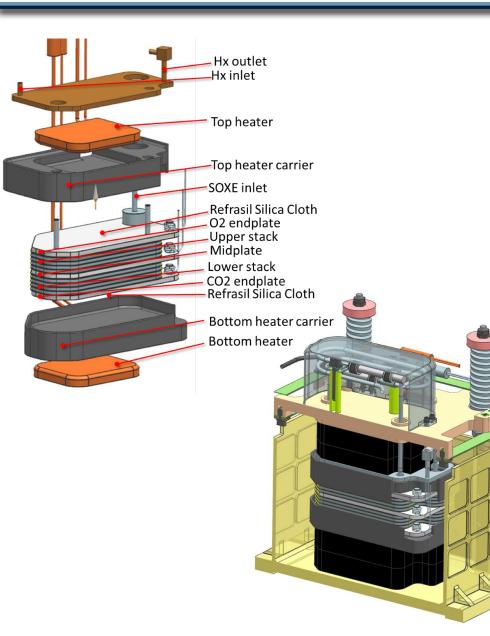
• Single cell with electrolyte layer • Stress distribution

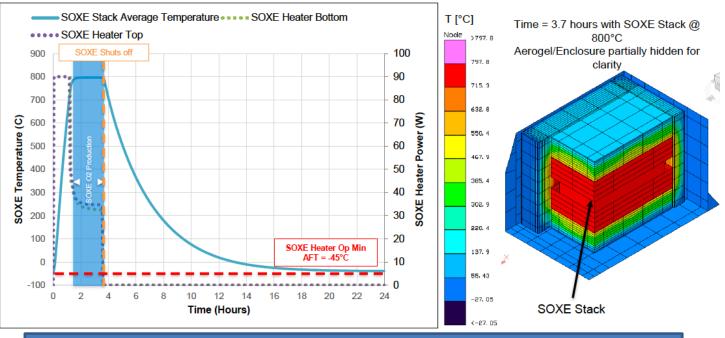






Thermal Analysis of MOXIE SOXE Stack





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)

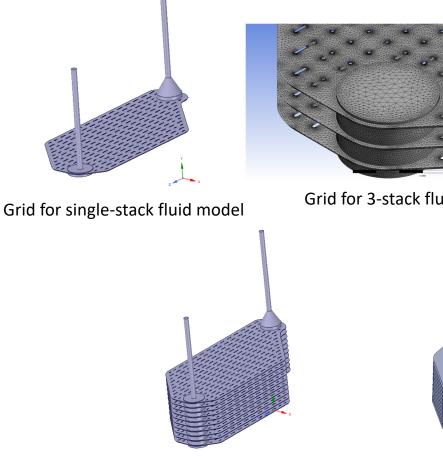
• SOXE Heat Leak during O2 production ~70 W

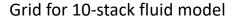
SOXE Min Op AFT of -45°C, SOXE average temperatures drops to -36°C after SOXE shuts off



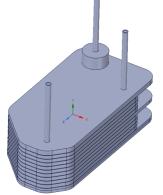
NASA Internal Future Modeling Directions

- 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 ٠
 - Obtain actual thermal and mechanical ٠ 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 3-stack fluid model



10-stack fluid model



- 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
 - CO₂ reduction cathode degrades without CO in dry CO₂.
 - Anode (delamination of electrode layer under high current density, high ionic O²⁻ flux).
 - Carbon deposition (coking) at high CO/CO₂ gas ratios. (Limits CO₂ 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.

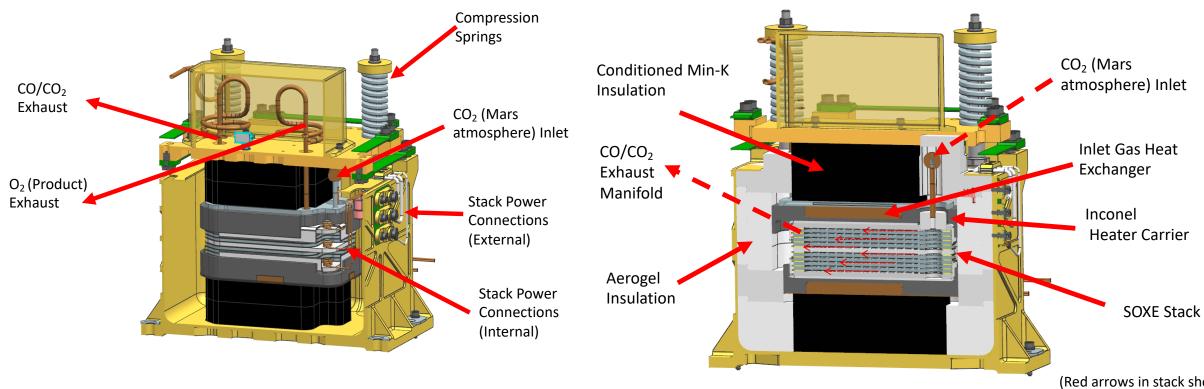


- Packaging
 - Insulation
 - Uniform insulation around stack capable of withstanding launch/landing vibration
 - Compression
 - Maintaining uniform compression to ensure sealing and electrical conductivity throughout stack
 - Accommodating instrumentation
 - Incorporation of adequate connections for 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



- 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





(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 O₂/hr
 - Manned Mission requires 2.2. kg of O₂/hr



- 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



- Benefits
 - Solid Oxide Electrolysis has higher utilization efficiency compare to lower-temp technologies
 - SOE generates dry-O₂ from various feedstocks (dry-CO₂, CO₂ + H₂O, and H₂O)
- 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