Solid Oxide Electrolysis Calibration and Characterization for MOXIE

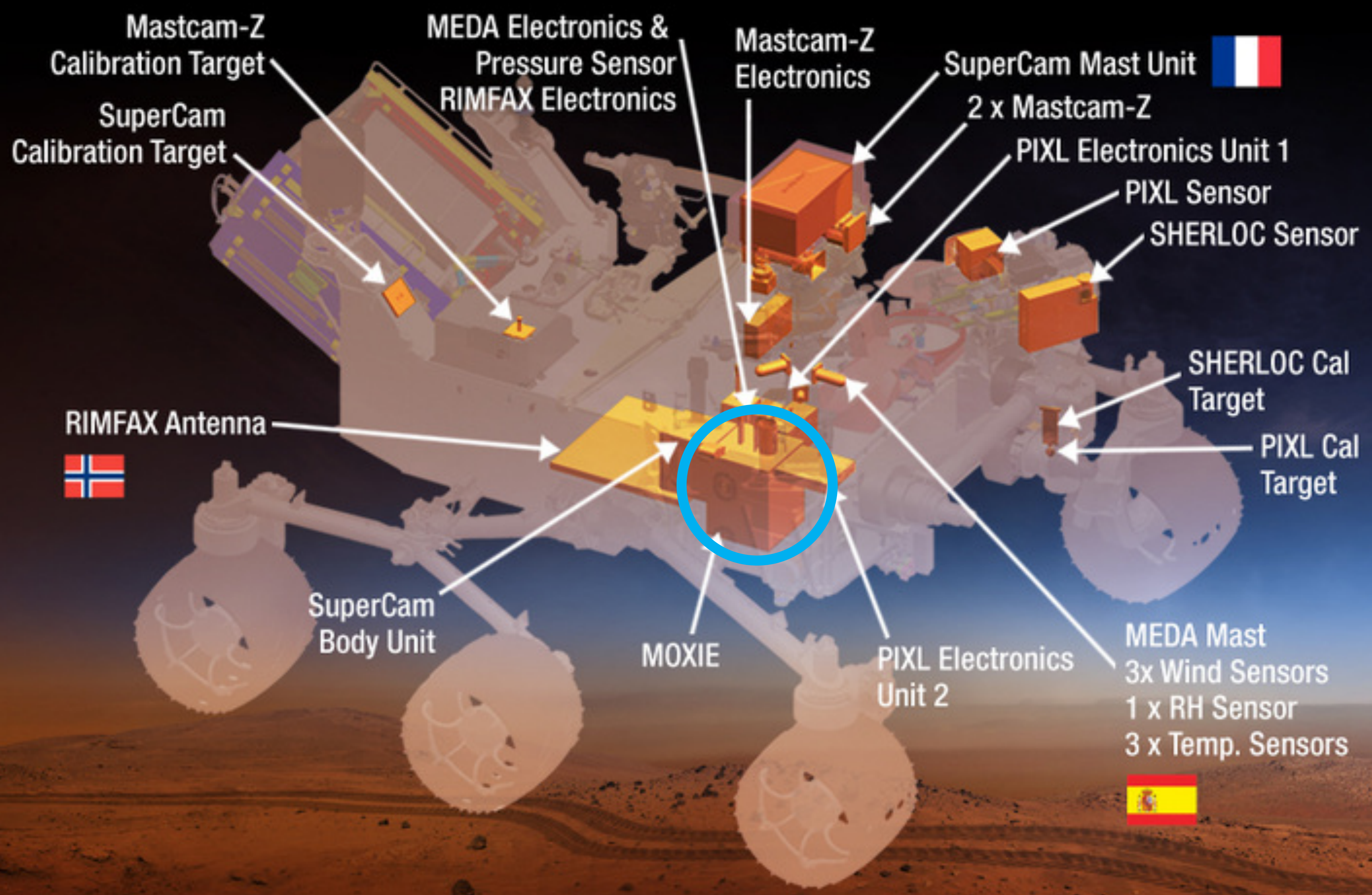
An Overview

Forrest Meyen and the MOXIE Team
2018 Space Resources Roundtable
June 13th, 2018

Mars 2020 Rover

Outline

- MOXIE Introduction
- C&C Background
- Characterization
- Calibration
- Next Steps



Introduction to MOXIE

Getting home from Mars

- The cost for a return trip from Mars is astronomical
- Enough for some to consider making a one way trip
- 30 – 37.5 mT of propellant needed for Mars Ascent Vehicle for a 4 - 6 person crew (Drake 2014, Polsgrove 2015, Rapp 2015)
- Ratio of mass in low earth orbit (LEO) to landed Mars mass is about 12:1 (Rapp 2015)
- 4-6 SLS launches needed just for propellant depending on payload configuration

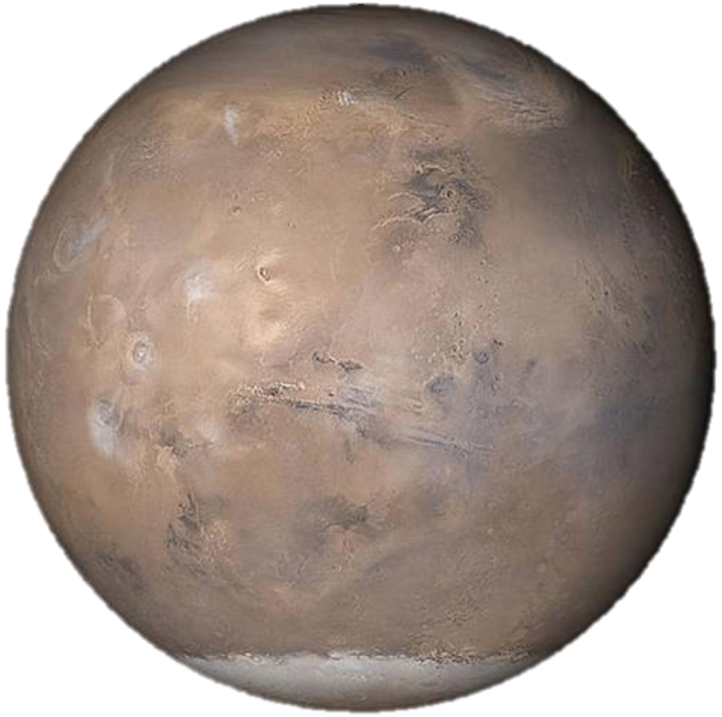
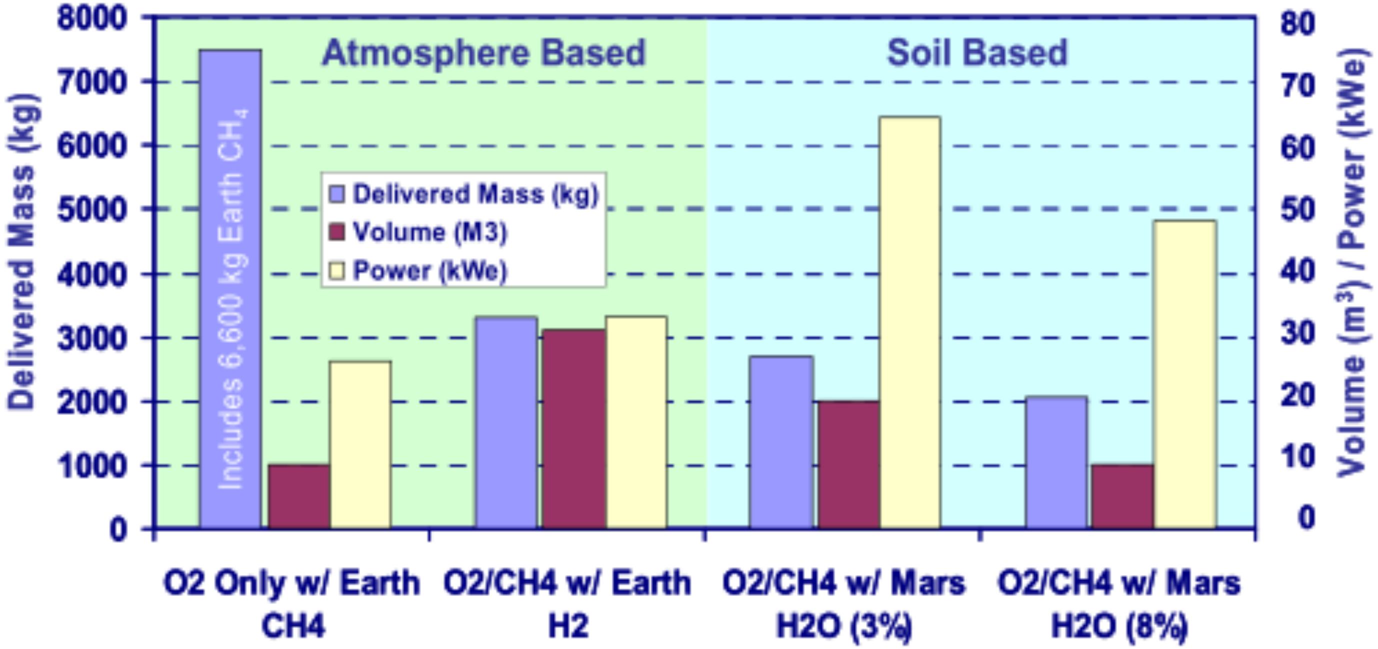


Image credit NASA/JPL-Caltech/MSSS

ISRU: An alternative to taking it all with you

- Oxygen alone is 78% of total propellant mass (for LO2, CH4)
- The MOXIE approach is the simplest way to use ISRU for propellant…

Les Bossinas 1989



Drake (2009)

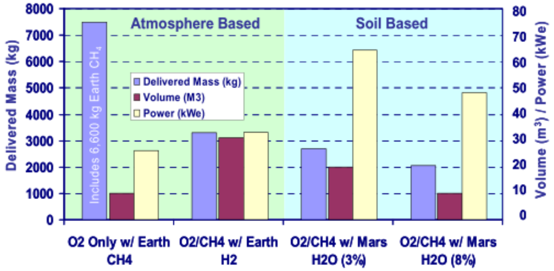
Any type of ISRU makes a major impact

… doing nothing requires an additional 4 large-sized SLS launches!

MOXIE technologies are applicable for soil and atmospheric based approaches

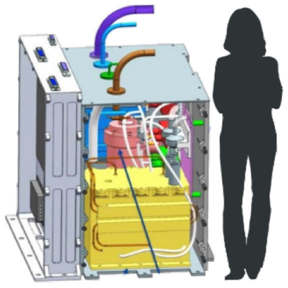
Without ISRU (~35 MT)



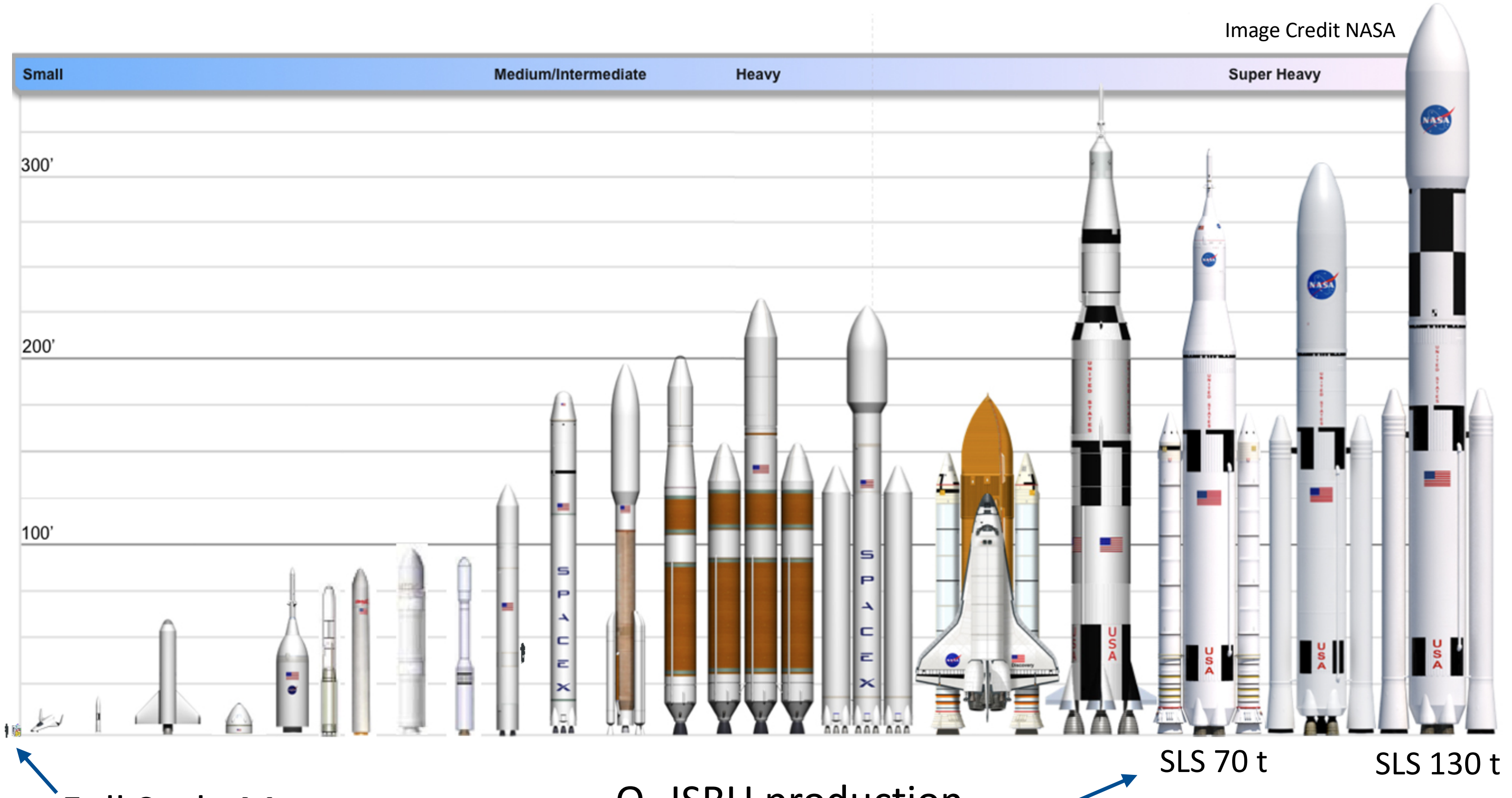



MOXIE – A scalable ISRU solution

MOXIE



Full Scale Mars Electrolysis Plant



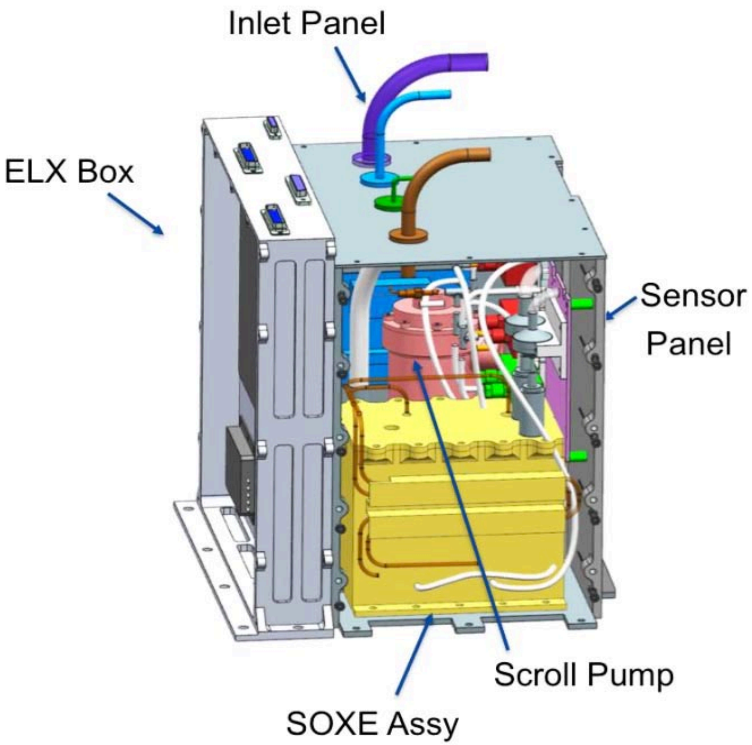
SLS 70 t

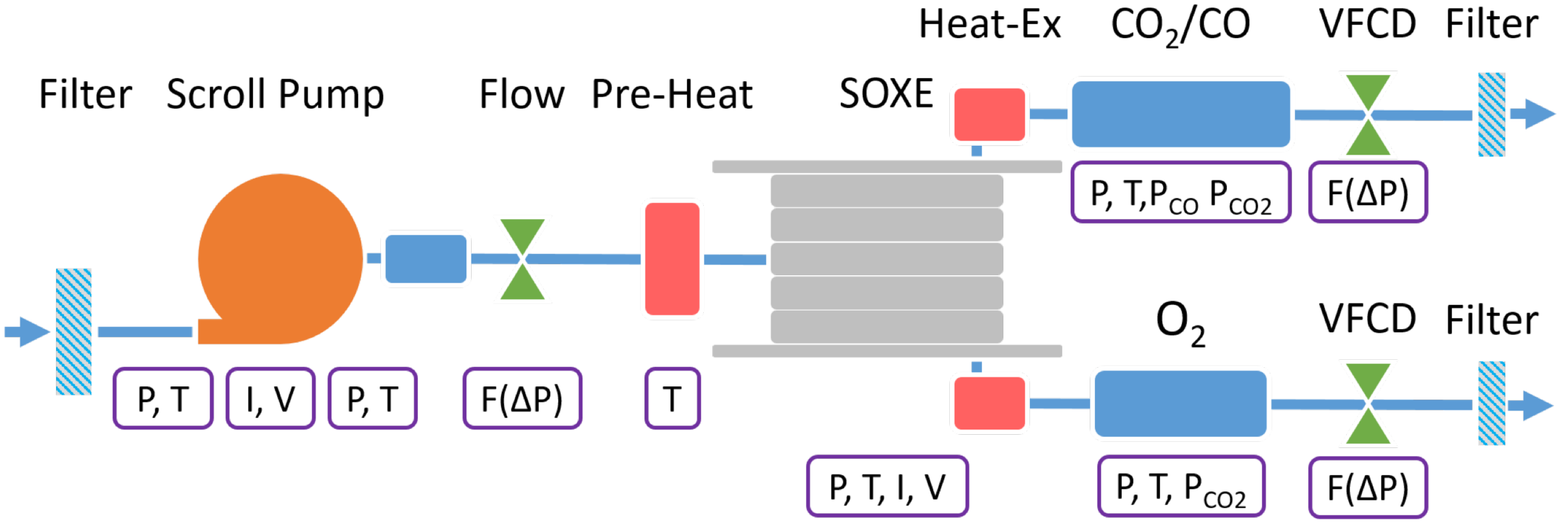
SLS 130 t

Full Scale Mars Electrolysis Plant

O_2 ISRU production replaces 4-5 of these

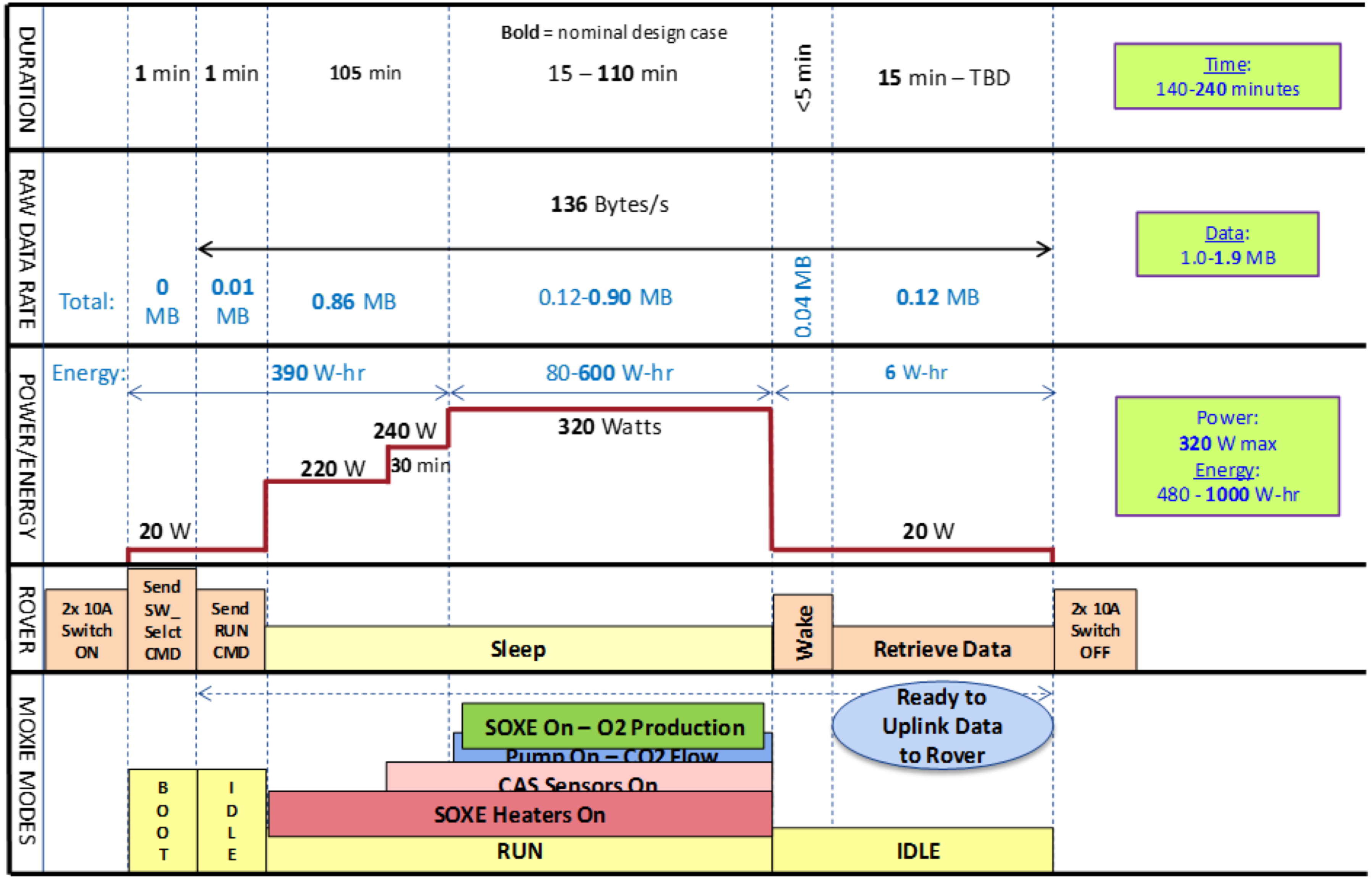
MOXIE Overview





Meyen (2015)

O_2 Production Resources



MOXIE as of June 2018

Calibration and Characterization Background

Definition: Calibration

- Measurement of unit-specific properties
  - Done on all units, but plan emphasizes flight model
  - Cannot use engineering unit as proxy for flight unit (by definition, that would be characterization)
  - Typically becomes part of archived data (PDS)
  - Valid only over tested ranges for limited time
- Typically links raw quantities to physical quantities
- Different methods may be used:
  - Reference to external standard (e.g. temperature of phase change)
  - Reference to known environment (e.g. pressure in vacuum)
  - Reference to well-characterized sensor (e.g. NIST-traceable)
  - Reference to other sensors of same or different type (last resort)

- Responsibilities
  - Science Team
    - Collaboration w/ Project on development of collaboration protocols
    - Calibration in cruise and on Mars
    - Production of calibration data products
  - Project
    - Calibration (and documentation) through ATLO

Definition: Characterization

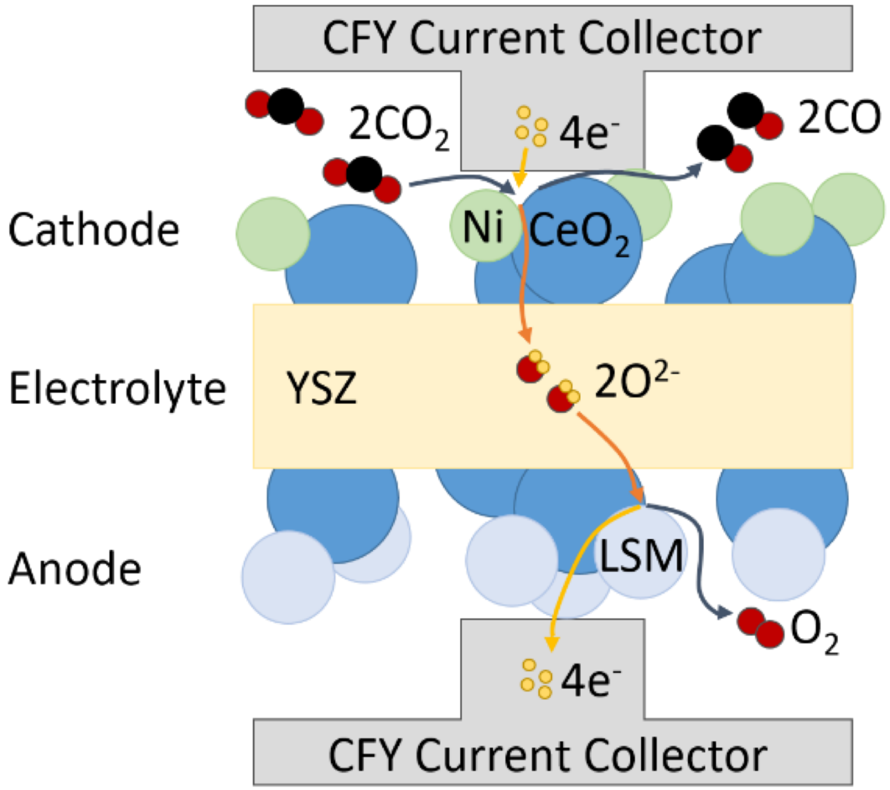
- Captures *general behavior* of component or system
  - Usually can be done using engineering models or system
  - Best done many times, in multiple labs, for extended time and with many variations
  - Describes most operations to date in MDTB (MOXIE Development Testbed)
  - Captured in reports, publications
- Serves various purposes for MOXIE
  - Planning and diagnostics during MOXIE operations
    - Understanding of safe and efficacious performance limits
    - Validation of command sequences, run tables, control algorithms
    - Debugging of faults and anomalous behavior
  - Refinement of analytical and numerical models
  - Guide to data interpretation
    - Recognition of idiosyncratic behaviors
    - Replication of measured performance
  - Studies of MOXIE performance beyond what we can do on the rover
    - Extended operation (target 1200 hrs.)
    - Controlled environments, e.g. dust, low temperatures, low elevation
    - Novel control schemes

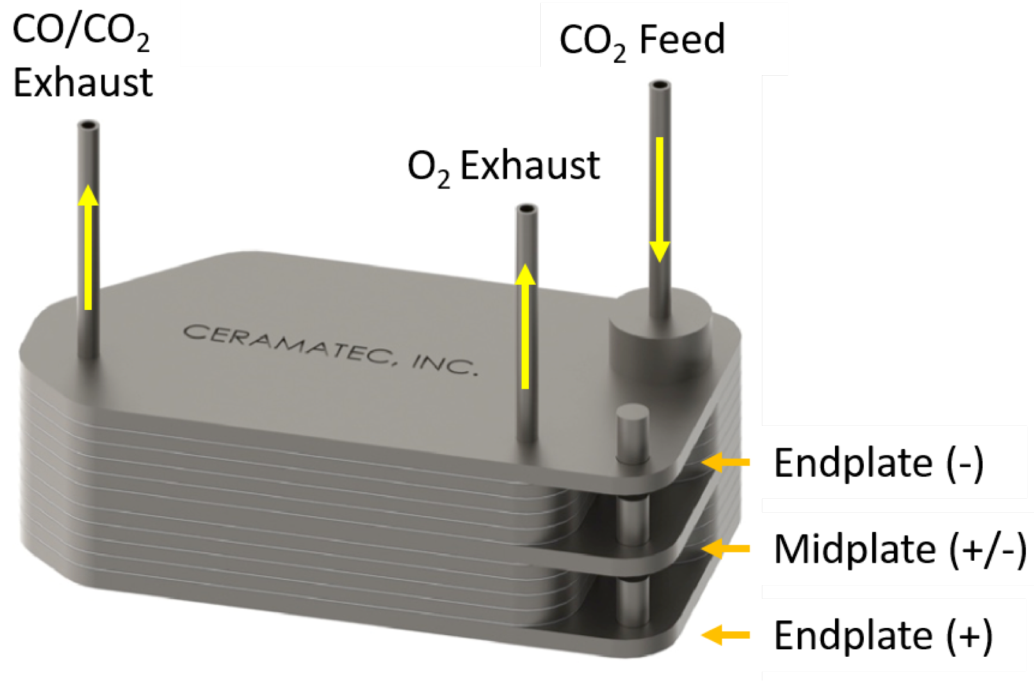
- Responsibilities
  - Science Team
    - Development phase studies complementary to MDTB activities
    - Increasing responsibility post-delivery
    - Everything subsequent to ATLO
  - Project
    - Build and operation of MDTB for V&V, troubleshooting, etc.
    - Tracking of FOMs during development phase

Calibration and Characterization Plans

- Plan broken into several C&C plans
  - Integrated System
  - Sensors
    - Temperature, pressure, voltage, current, flow, composition (CO CO_2 O_2)
  - Flow
    - Carbon dioxide acquisition and compression
    - Pump performance, pressure control (Viscous flow control devices)
  - SOXE (Today)
    - Electrochemical performance and modeling

Enabling Technology: Solid Oxide Electrolysis



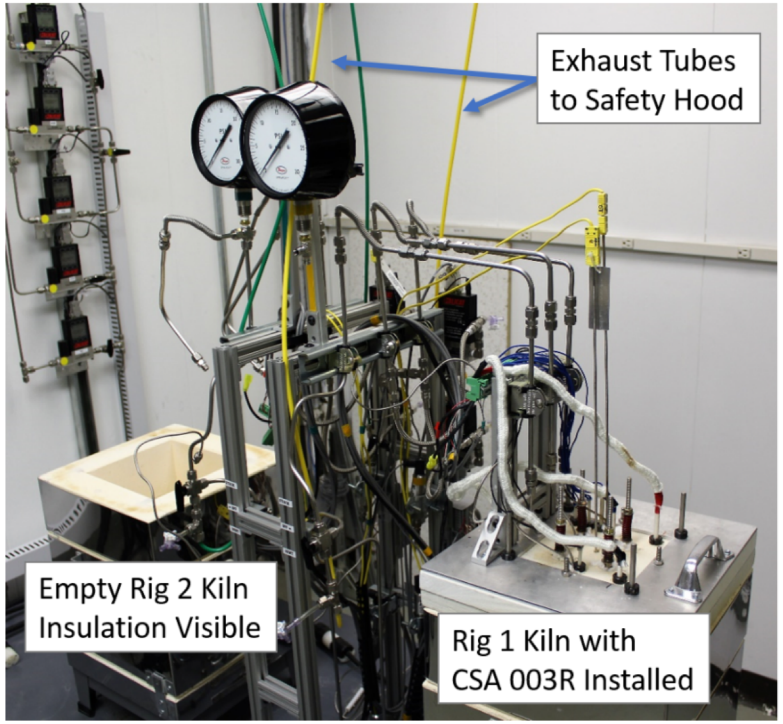


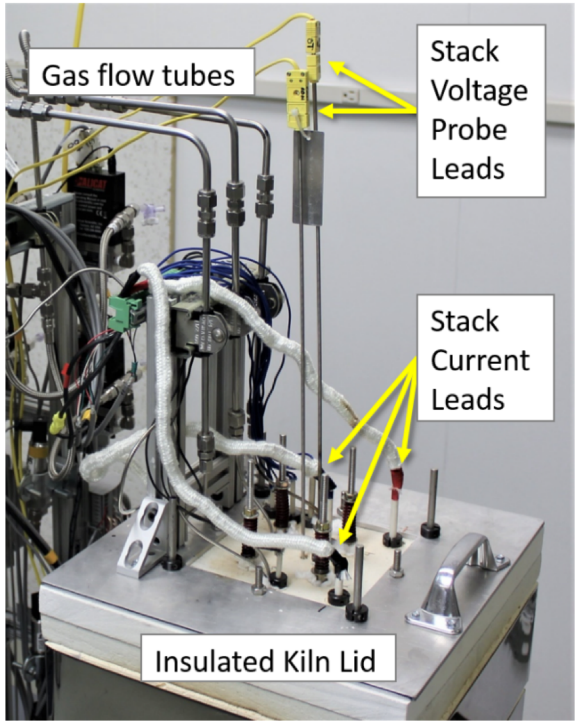
SOXE Characterization

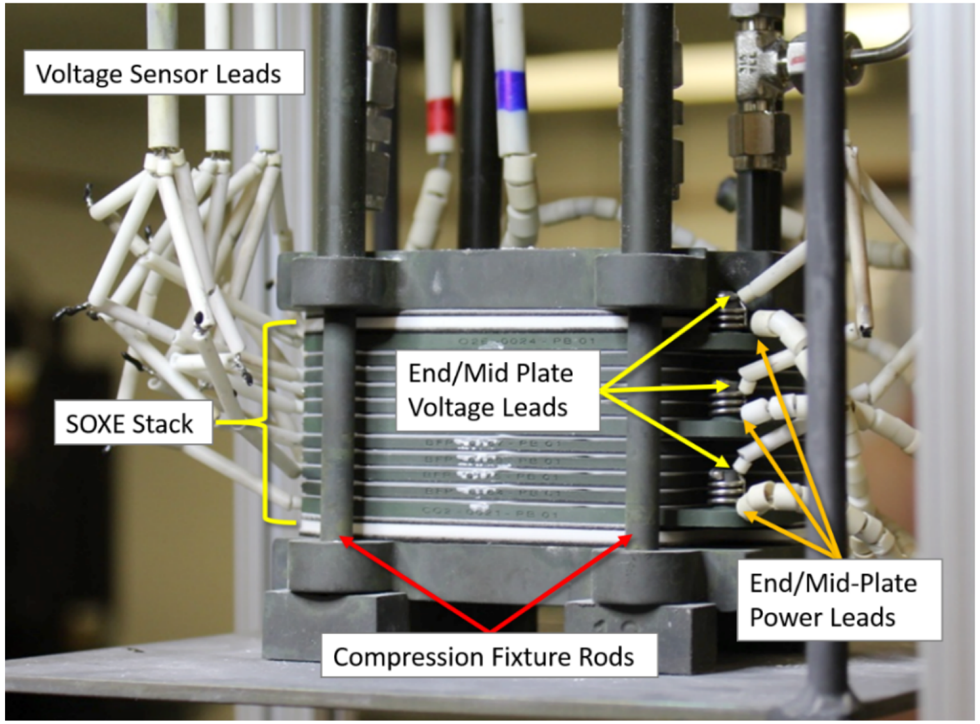
Characterization Facilities

- Laboratory facilities
  - SOXE Testbed at Ceramatec
    - Supported through SOXE Delivery to JPL
  - MOXIE Development Testbed (MDTB) at JPL
    - Supported through MOXIE delivery
  - MOXIE FlatSat Testbed at MIT
    - Chamber to be purchased and configured
    - Inherits some hardware & software from MDTB
    - Location Bldg. 37 (Man Vehicle Lab)
  - MOXIE EM test chamber
    - Co-located in Bldg. 37
  - MOXIE Sensor test chamber
    - Co-located in Bldg. 37
  - Other Co-Investigator Lab facilities in U.S. and Europe
    - Occasional use of Aarhus wind tunnel, JSC racetrack tunnel
- Hardware
  - SOXE stacks
  - MOXIE FlatSat
  - MOXIE Engineering Model (EM), spares, and ground support equipment (GSE)
  - Component and subsystem-level MOXIE hardware (e.g. sensors)
- Software
  - Ability to simulate flight software environment for validation
  - LabVIEW, Simulink, or custom software
  - In-house ability to modify 8051 software
- Performance models
  - MATLAB/Simulink, Excel

Characterization Facilities: Ceramatec SOXE Testbed



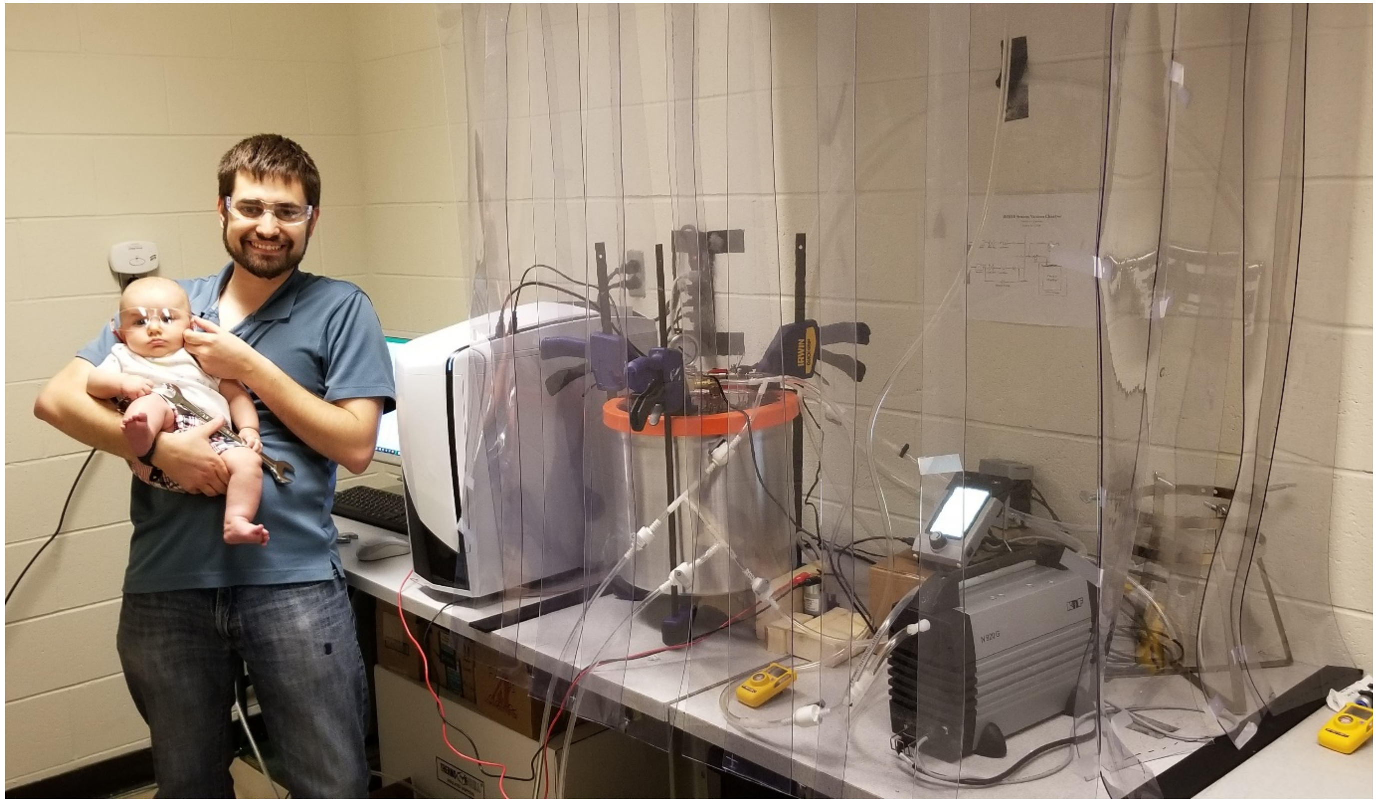




SOXE Test Environment independent of other subsystems (Retired)

Characterization Facilities: JPL MDTB

Characterization Facilities: MIT Sensor Testbed



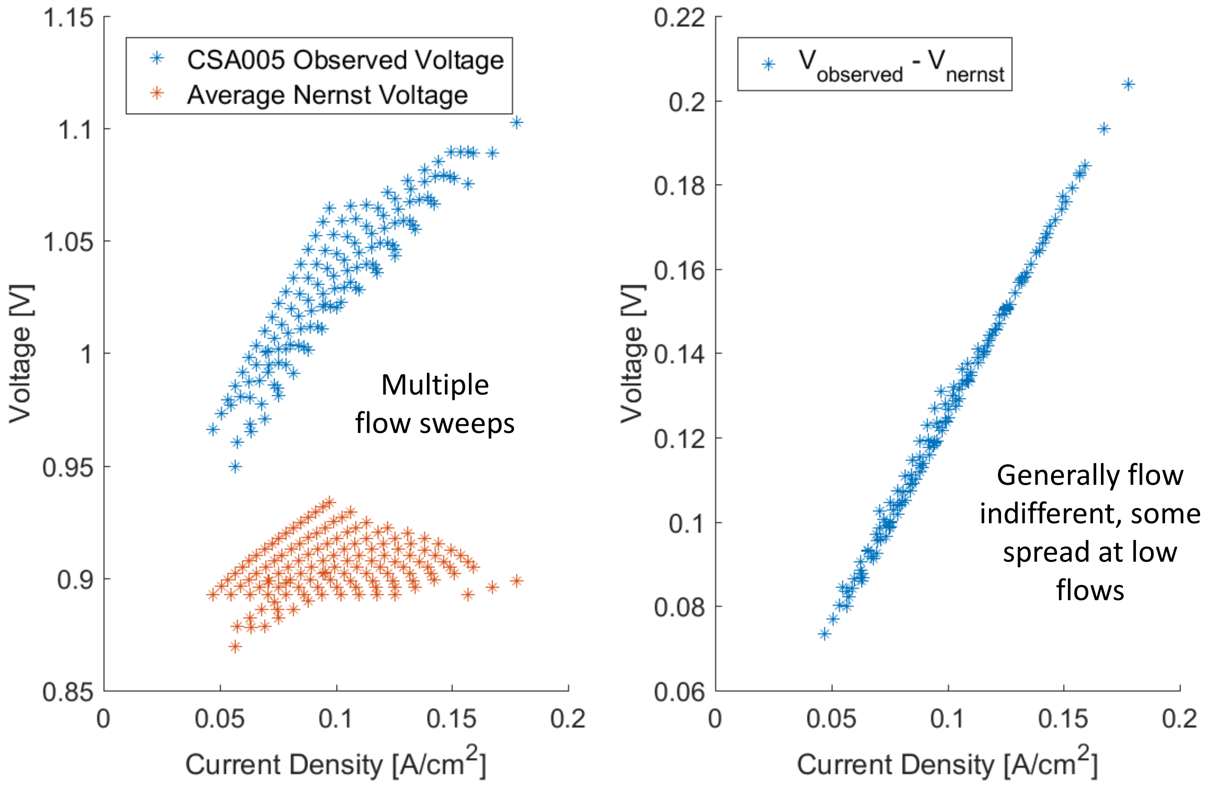
MOXIE Sensor Test Lab at MIT, to be expanded to MOXIE Engineering Model Testbed

Characterization Activities

1. SOXE stack performance dependence on operational parameters (I, V, P, T, m)

2. Transient oscillation effects (flow and power) – In Progress

3. SOXE stack degradation and lifetime (and resulting models)
   a. Operational Limits
   b. Dynamic Limits



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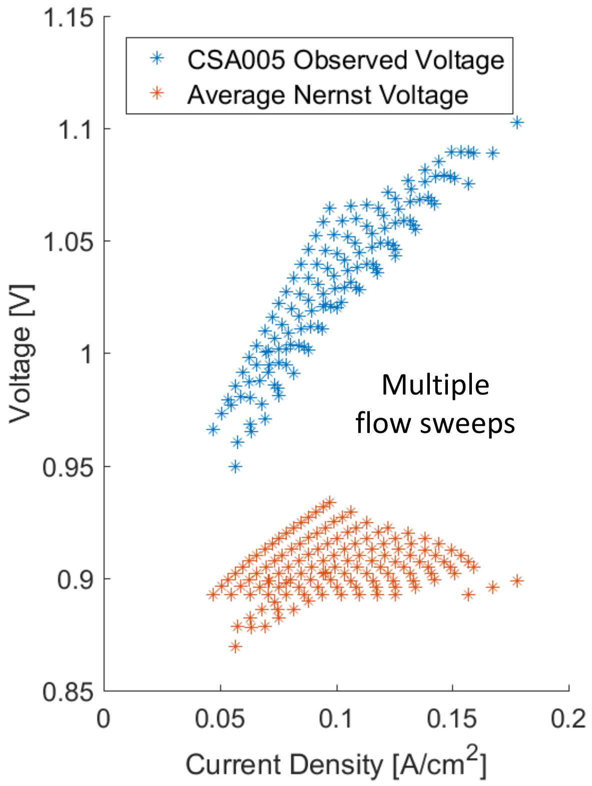

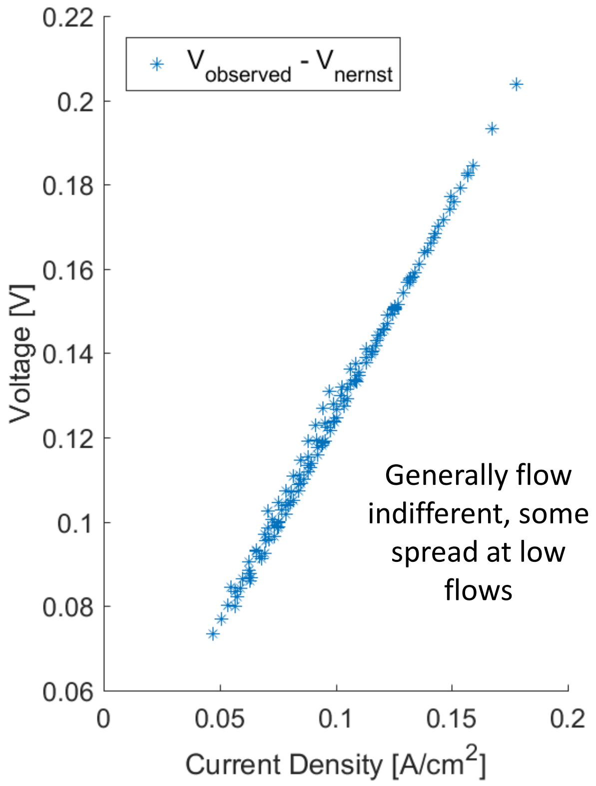

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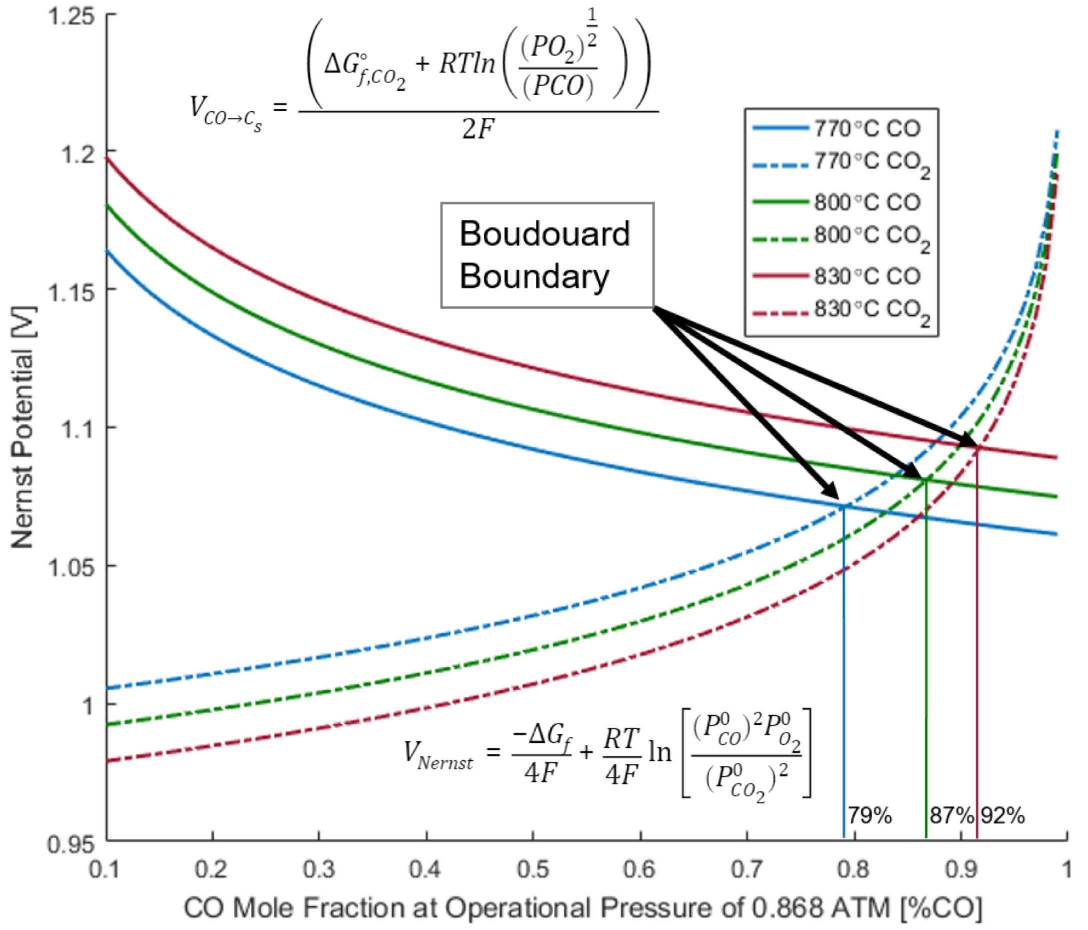

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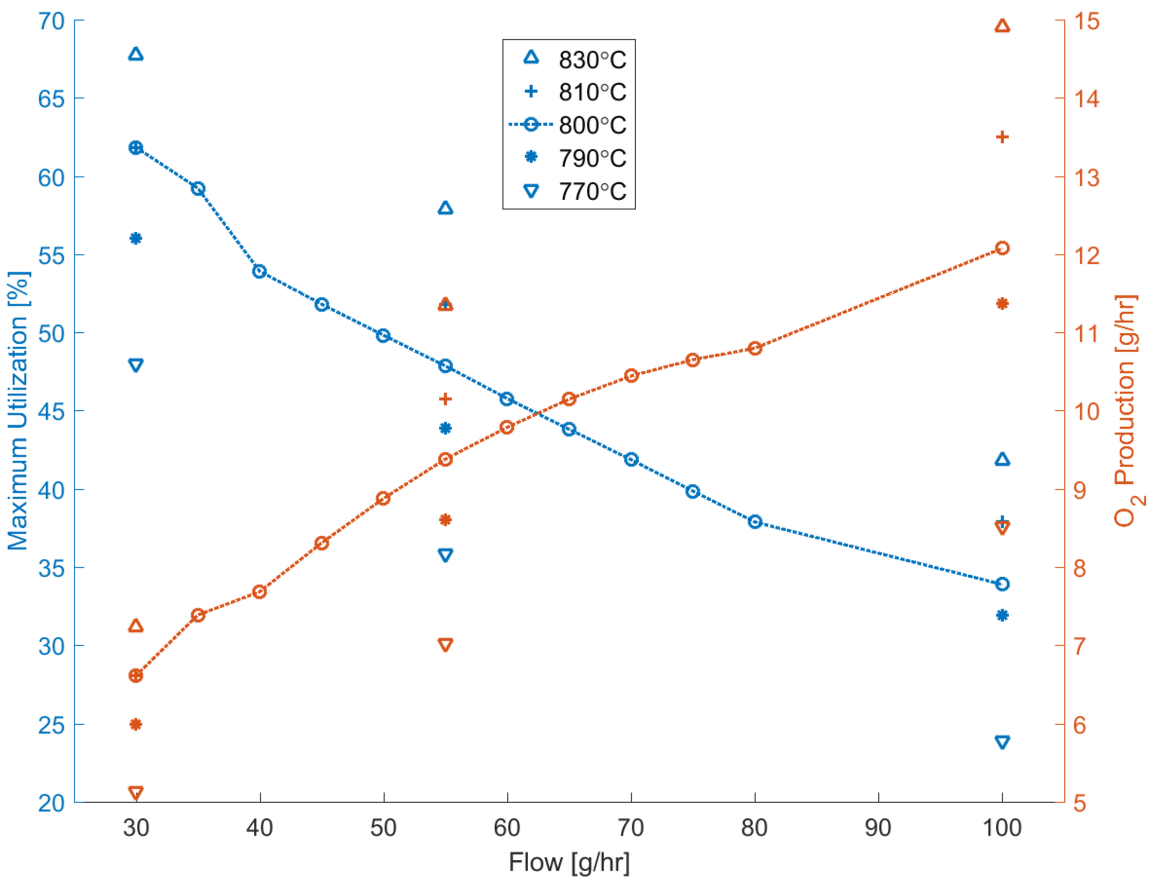


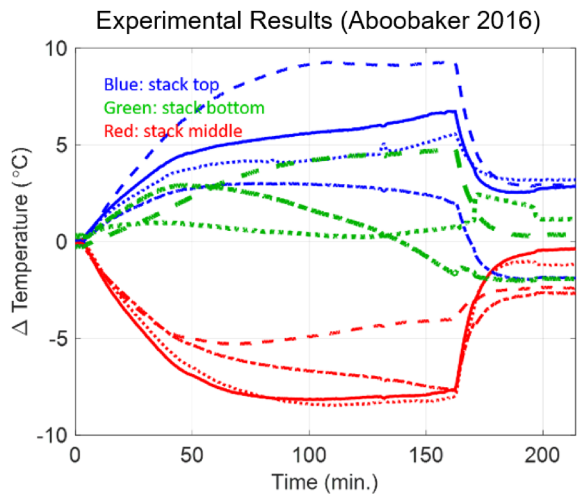
Characterization Activities

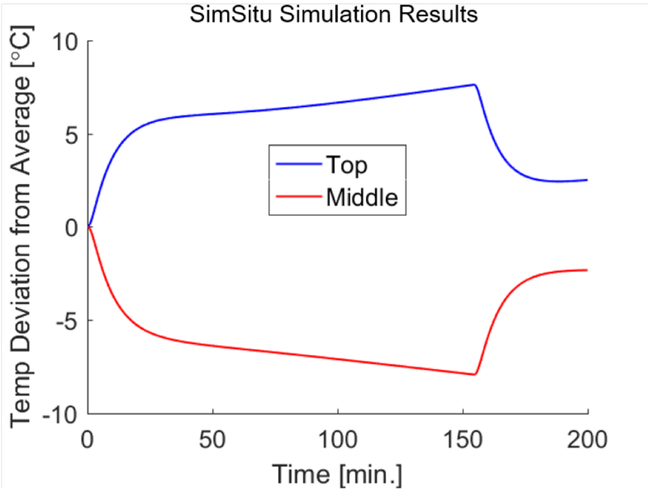
4. SOXE thermal characterization
   - Temperature distribution between cells for all operational states

5. Voltage uncertainty
   - Amount of voltage loss over the leads to the SOXE

6. Cell-cell performance variation trends relating to flow

7. Sensor error, accuracy, and expected drift (to be provided by Sensor C&C)





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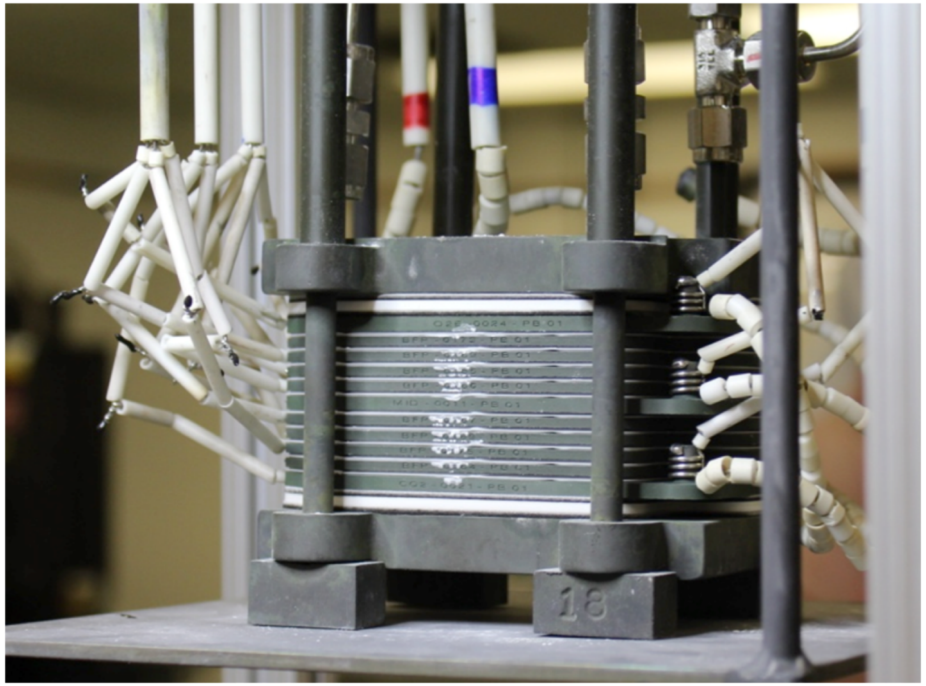

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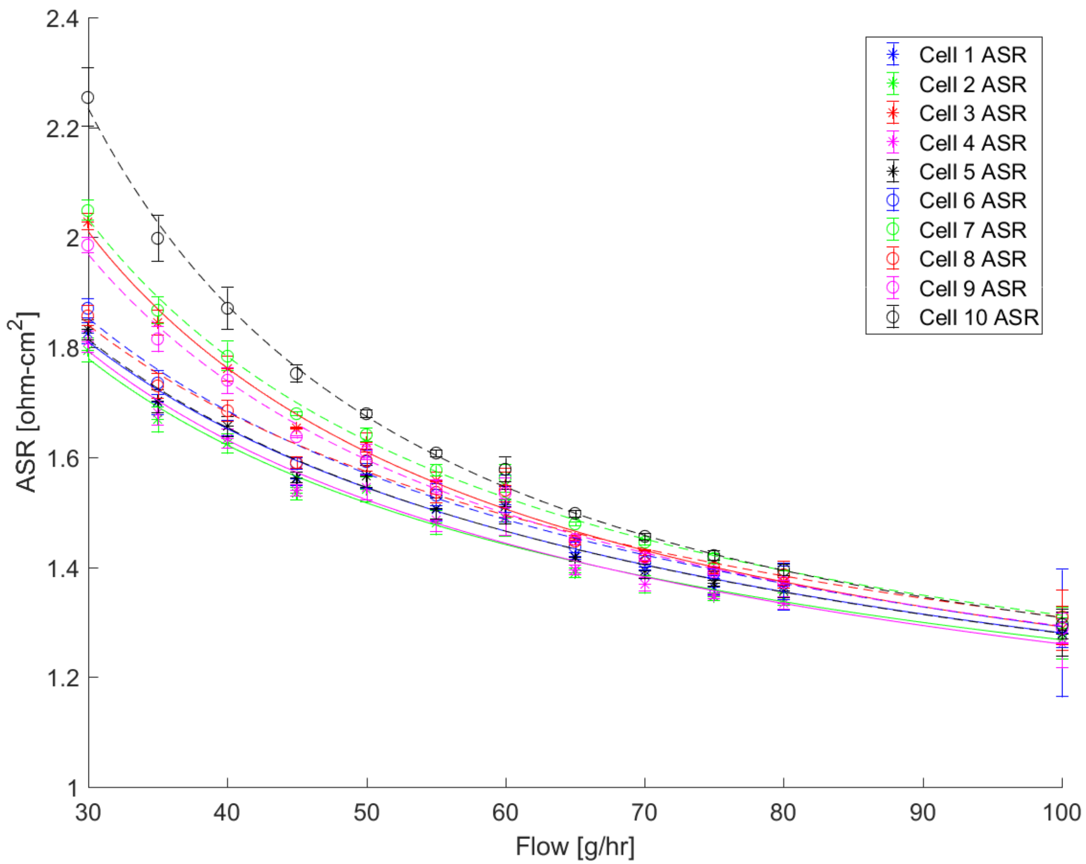

Development cell CSA 005

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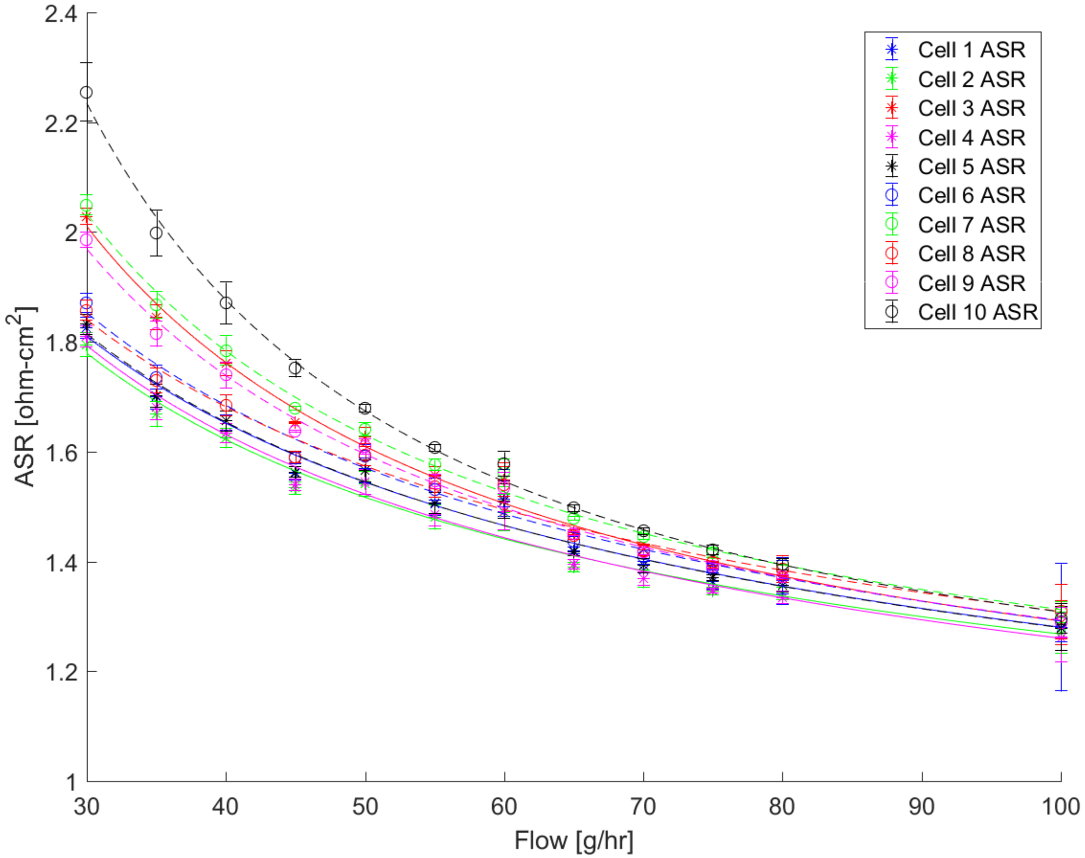


Development cell CSA 005

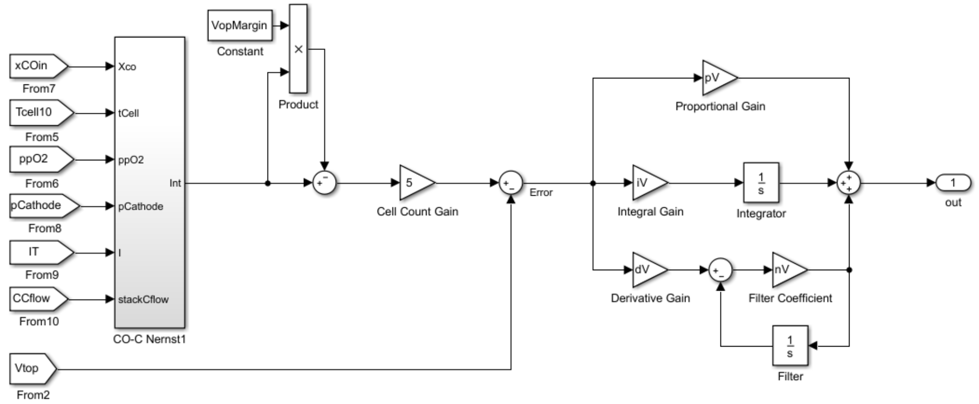
Characterization Activities

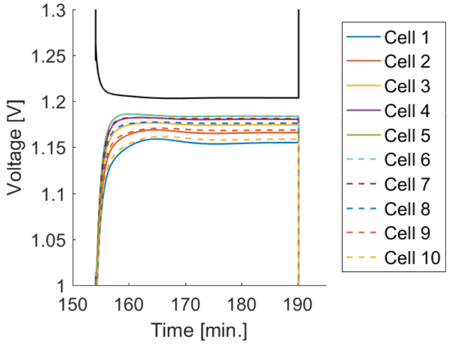
8. SOXE control system characterization

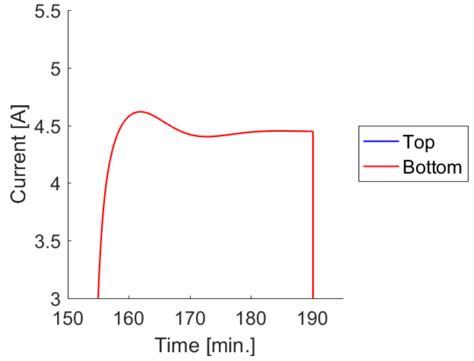
9. Characterize the effect of flight instrumentation limitations on safe MOXIE operational command envelope

10. Fault detection isolation and recovery (FDIR)

11. Expected behavior differences in SOXE performance and safe operational limits between test setups







Includes evaluation of advanced control concepts

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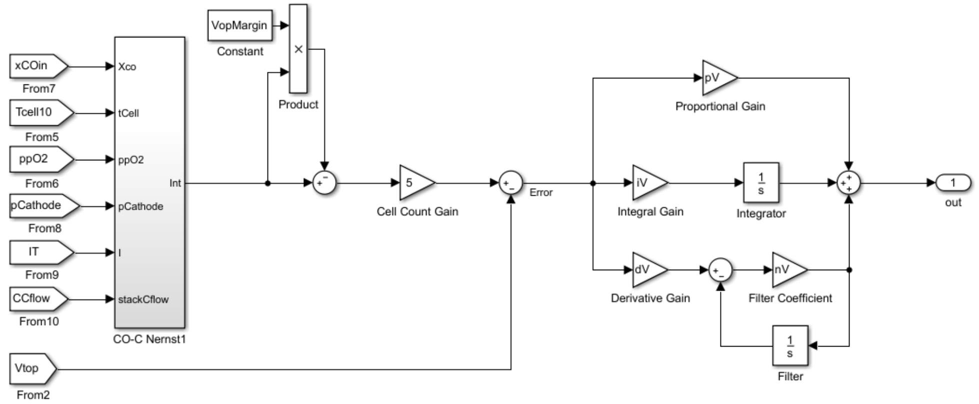

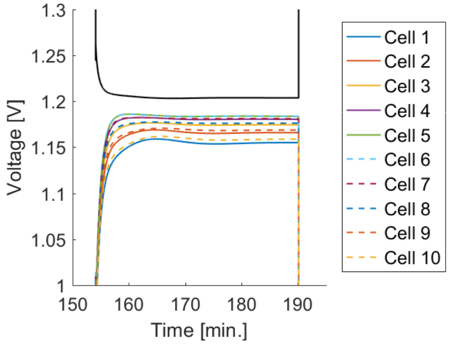

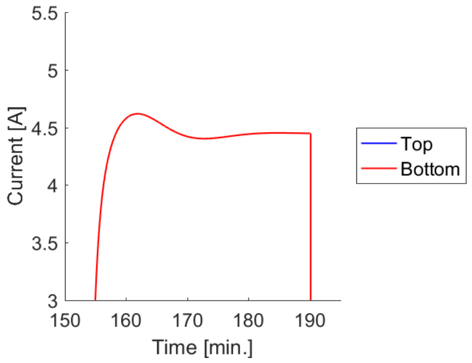

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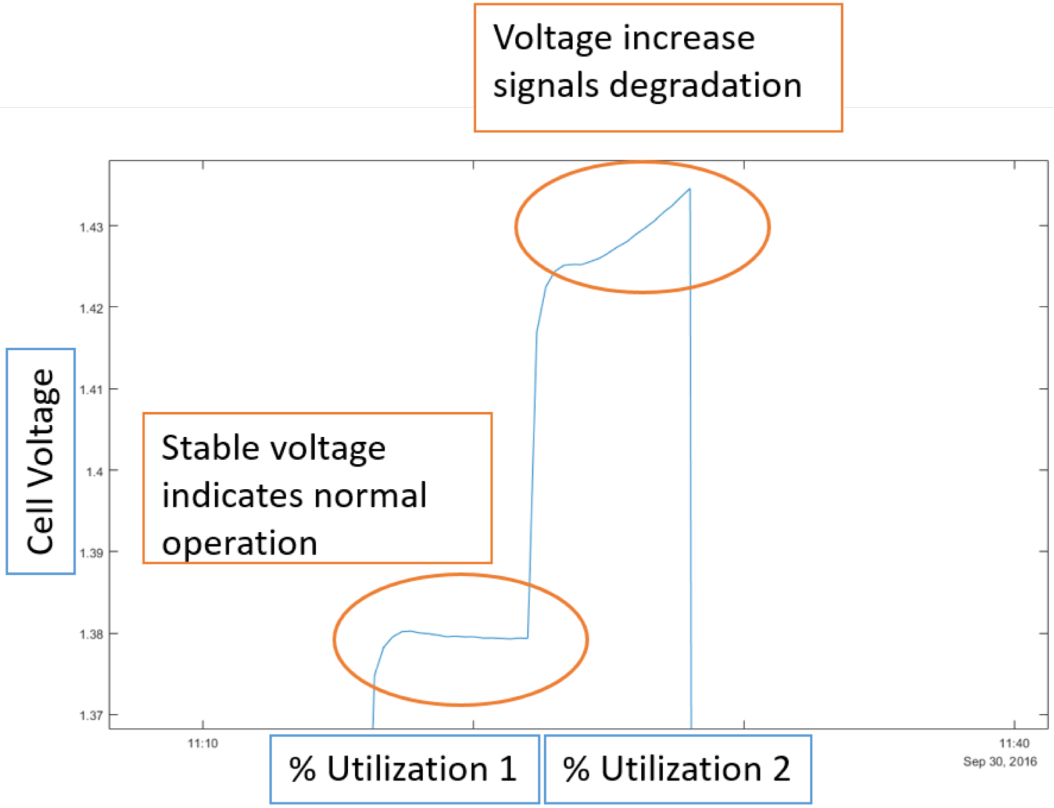

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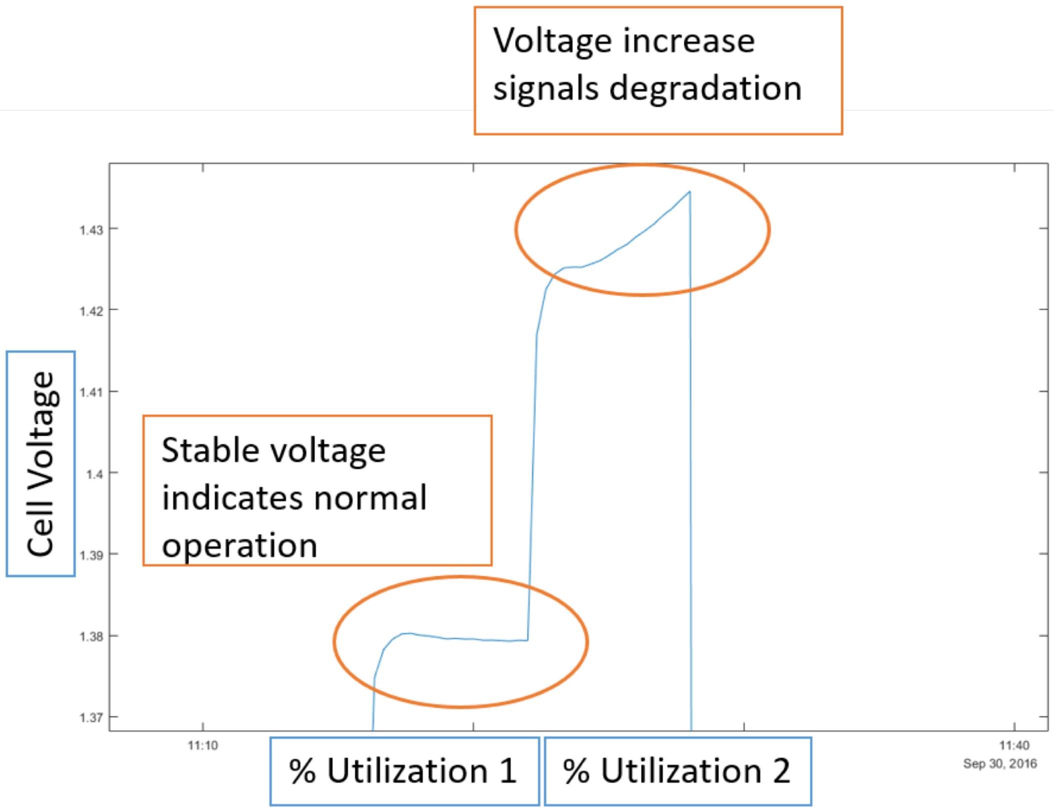


SOXE Calibration

Calibration Topics

1. Performance Calibration Mapping
   a. i-V Sweeps
      - Derived terms
        - ASR
        - i-V intercept
        - Conversion Corrected ASR
        - Activation potential

   b. Stack flow sweeps
      - Derived terms
        - Intrinsic ASR
        - Activation potential
        - Conversion Corrected ASR flow correction term (model enhancement)

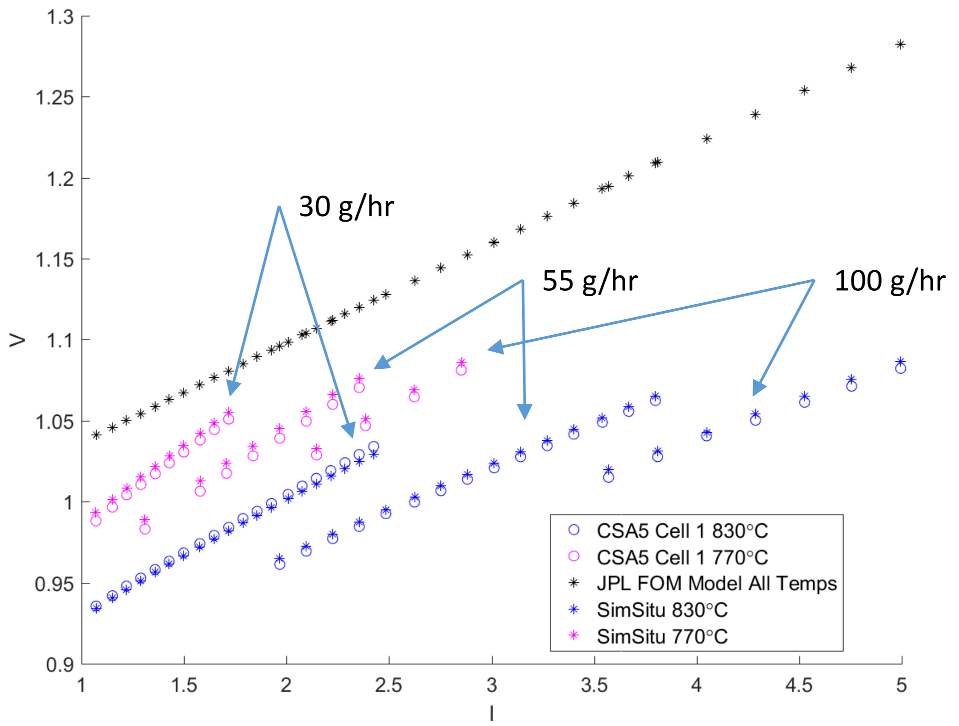
   c. Open circuit voltage reference
2. Stack gas leak rate check
   a. Check at Ceramatec and after acceptance at JPL (after operational cycle 2)
3. Stack Lead wire resistance
   1. Calibrate for each stack and check for changes over time

Tuned models build understanding

$$V = V_{act} + V_{Nernst,CO2-CO} + I\left(ASR_{cc} * \frac{1}{Ae^{\left(\frac{E_a}{RT}\right)}} / A_{cell}\right)$$

$$\overline{V}_{nernst} = \frac{1}{x_{co,out} - x_{co,in}} * \left[\frac{-\Delta G_f^o}{4F} x_{co} + \frac{RT}{4F}\left(x_{co} \ln\left(\frac{P_{O_2} * x_{co}^2}{(x_{co}-1)^2}\right) + 2\ln(1-x_{co})\right)\right]_{x_{co,in}}^{x_{co,out}}$$

- Model made from 20% of data
  - 100 g/hr only i-V sweeps at all characterized temperatures
  - Conversion correction accounts for flow variations in ASR for 30 and 55 g/hr tests
  - Arrhenius Relation accounts for temperature
- RMS Error still small at extreme limits
  - 0.0051 V for 770 °C
  - 0.0031 V for 830 °C

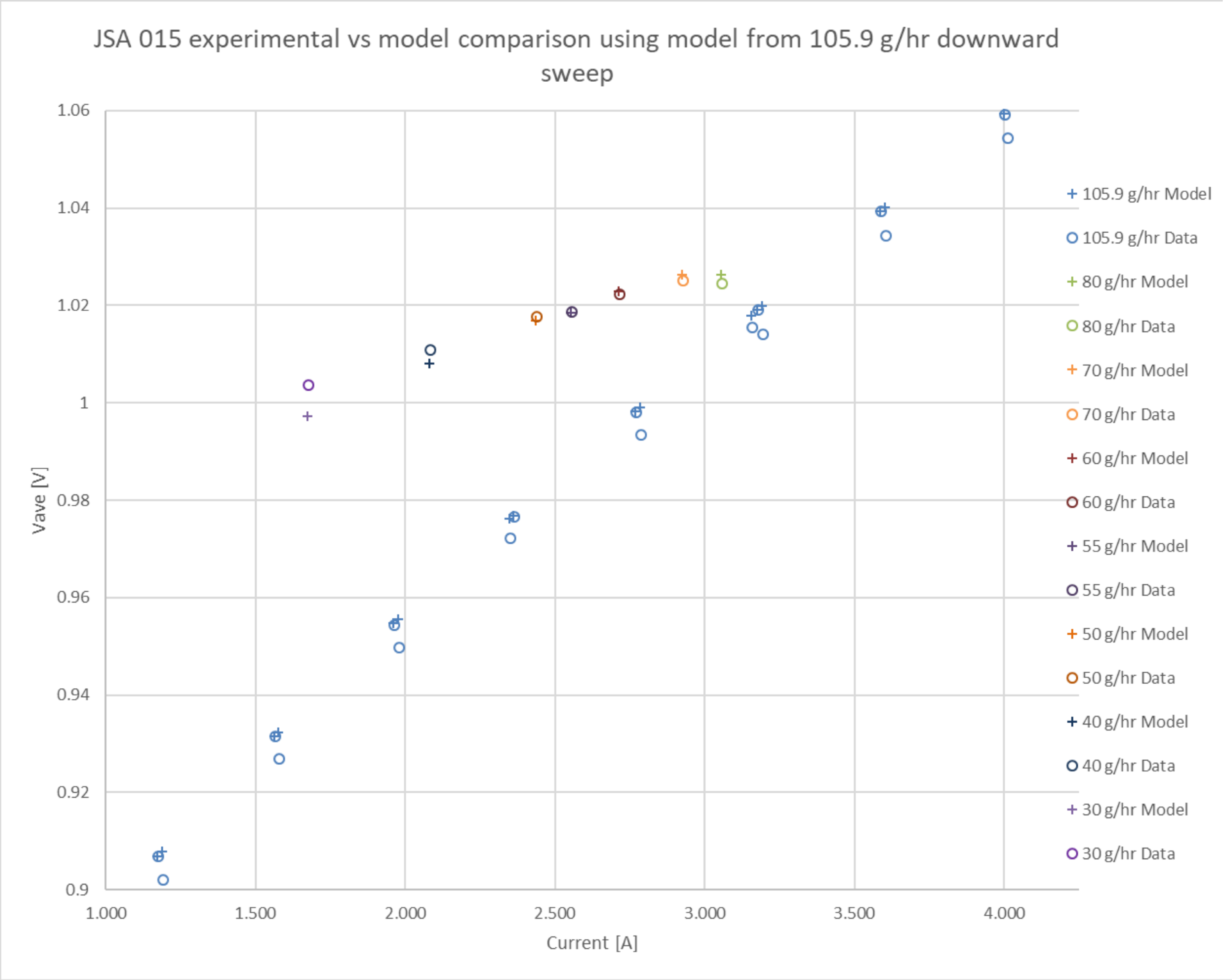


Performance Calibration Mapping

- Initial Calibration Approach (Operational Cycle 1 and 2)
  - Feed Gas CO_2 with 2% CO when not using recirculation
  - 800 C baseline temperature
  - i-V curve at 105.9 g/hr. with an upward and downward sweep
  - Flow sweep with single points sampled at 30, 40, 50, 55, 60, 70, 80, 105.9 g/hr
- Enhanced Calibration
  - i-V sweep at 30, 55, 80 g/hr.
- Basic calibration check (proposed)
  - Conservative i-V sweep at 55 g/hr., from 16% (1 A) to (2.3A) utilization
  - No open circuit voltage sample (unless 2% CO feed is available)

Baseline Calibration Flow Sweep

% CO_2 Utilization	Flow (g/hr)	Total Flow (sccm)	CO_2 Flow (sccm)	CO Flow (sccm)	Current (Amps)	Top Upper Voltage Limit (VDC)	Bottom Upper Voltage Limit (VDC)
26	105	898.4	884	14.2	3.158	7.674	7.685
33	80	678.6	667	11.2	3.059	7.658	7.667
36	70	593.8	583	10.7	2.928	7.577	7.584
39	60	509	499	10	2.719	7.426	7.428
40	55	466.6	457	9.4	2.558	7.300	7.300
31.4	55	466.6	457	9.4	2.000		
42	50	424.2	415	8.9	2.438	7.218	7.252
45	40	339.3	332	7.7	2.088	6.951	6.943
48	30	254.5	248	6.2	1.678	6.646	6.628



Fit using downward i-V curve. Some voltage gain between upward and downward 105.9 g/hr sweep.

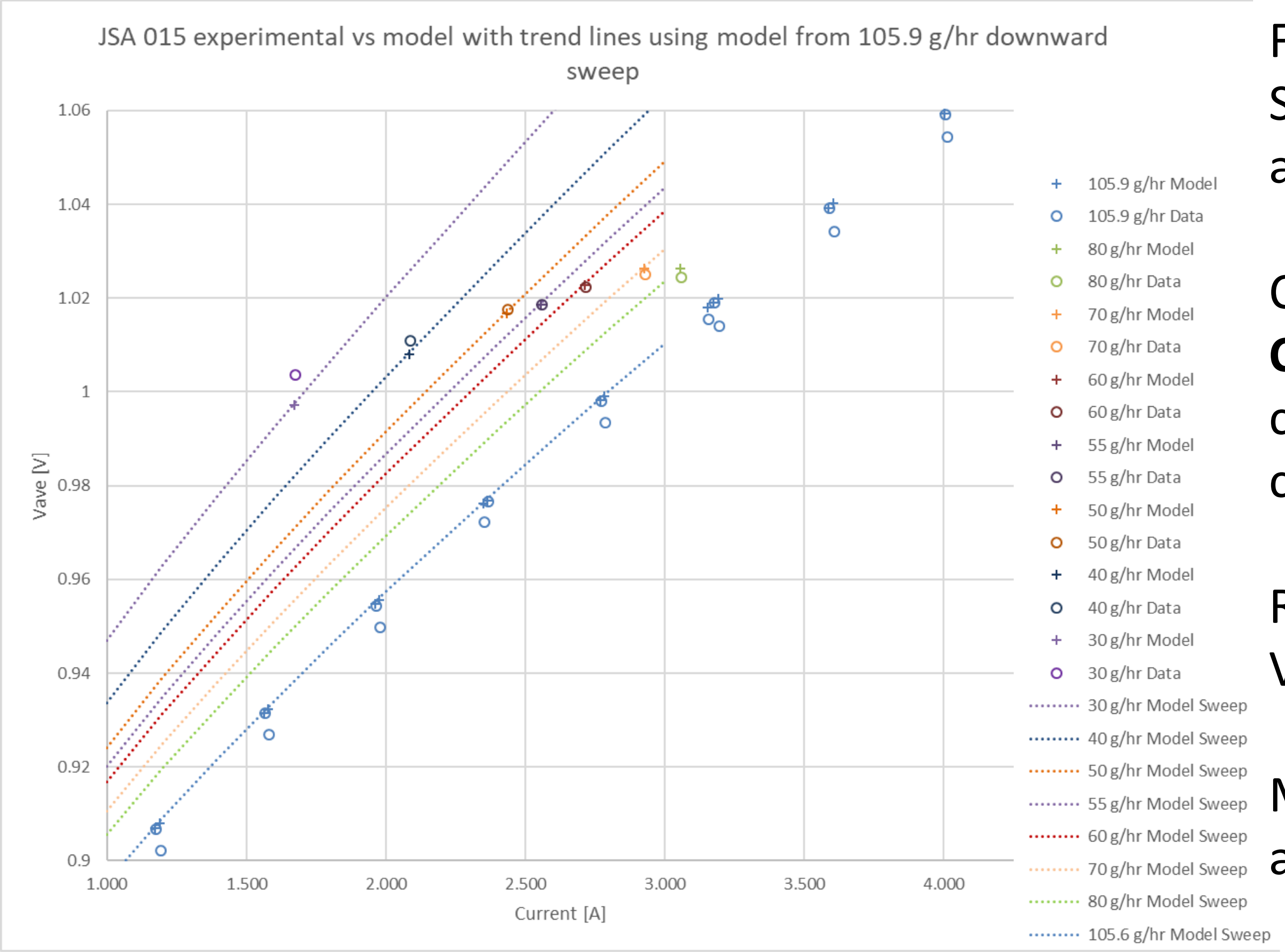
Comparison Using **Conversion Corrected** ASR

ccASR = 0.8088

ccVact = 0.022

RMS Error of Flow Points = 0.00099 V or 0.99 mV

Model **is very good** and only loses accuracy at very low flows.



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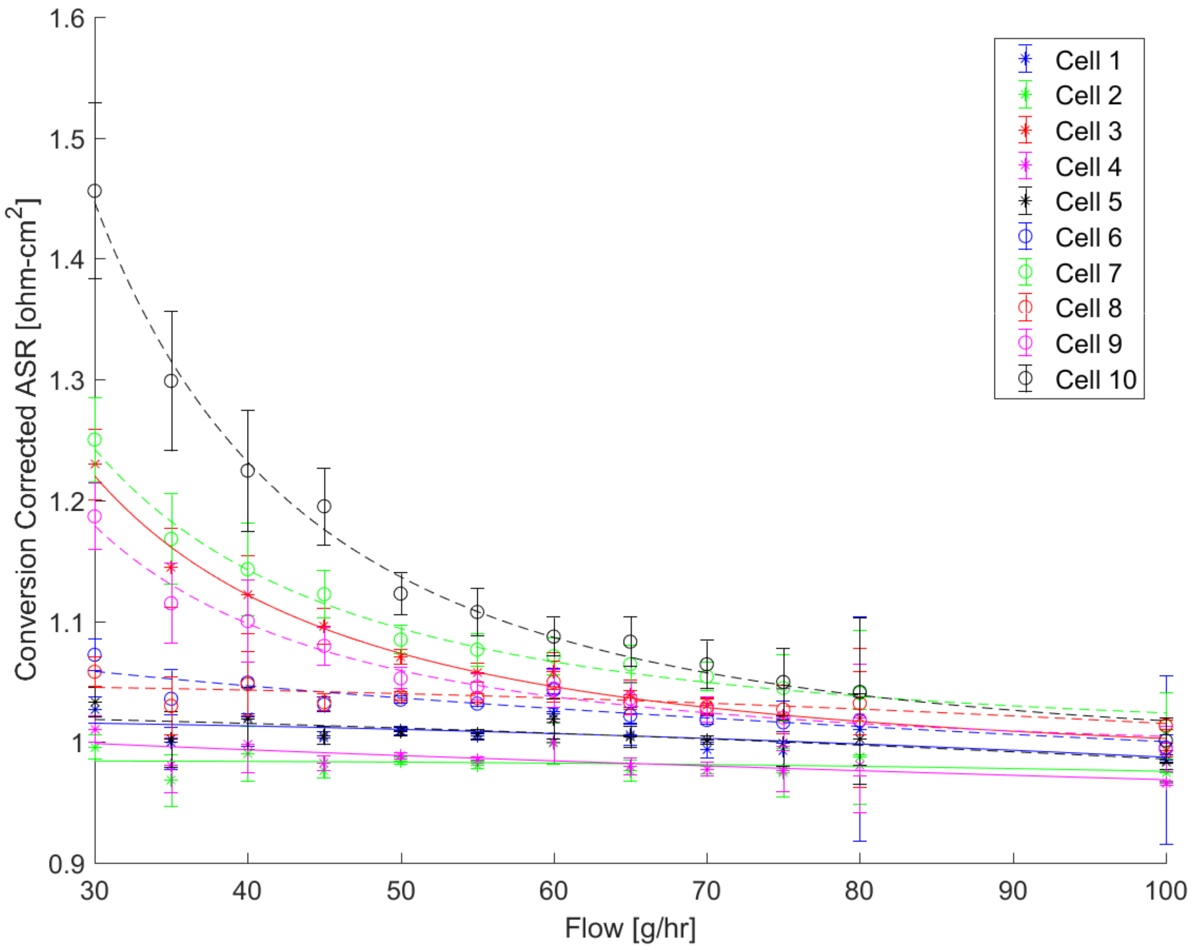
Previously characterized behavior

- Previous observed behavior of development stack shows deviation from ideal model at lower flow conditions
- New term proposed to tune the CCASR term for each stack



Enhanced Performance Mapping

Flow (g/hr)	Current (Amps)	Transition Time
80	2.059	30 min
80	1.059, 1.559, 2.059, 2.559, 3.059	30 sec each
80	3.059, 2.559, 2.059, 1.559, 1.059	30 sec each
80	2.059	15 min
55	1.758	30 min
55	0.958, 1.358, 1.758, 2.158, 2.558	30 sec each
55	2.558, 2.158, 1.758, 1.358, 0.958	30 sec each
55	1.758	15 min
30	1.278	30 min
30	0.878, 1.078, 1.278, 1.478, 1.678	30 sec each
30	1.678, 1.478, 1.278, 1.078, 0.879	30 sec each
30	1.278	15 min
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55	0.958, 1.358, 1.758, 2.158, 2.558	30 sec each
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55	1.758	15 min
80	2.059	30 min
80	1.059, 1.559, 2.059, 2.559, 3.059	30 sec each
80	3.059, 2.559, 2.059, 1.559, 1.059	30 sec each
80	2.059	15 min
	Total	4:10

- Enhances ground truth of model for prediction and planning
- Enables flow dependent Conversion Corrected ASR term
- Designed to minimize hysteresis and system effects

Calibration by development phase

- Component level calibration (At Ceramatec, fixed as OC1)
    - Flow sweep with single points sampled at 30, 40, 50, 55, 60, 70, 80, 105.9 g/hr
    - i-V curve at 105.9 g/hr with an upward and downward sweep
  - Quantify cell to cell voltage variation
- In MDTB at JPL
  - OC2 for comparison to OC1
  - Quantify cell to cell voltage variation
  - Enhanced Calibration Procedure
- In ATLO (As part of MOXIE and Mars 2020 thermal stress test)
  - Basic calibration possible
- In Cruise
  - Aliveness
  - No electrolysis operation possible
- On Mars
  - Basic calibration. Flow rate depending on landing site and environmental conditions

Acknowledgements

Special Thanks

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MIT HAYSTACK OBSERVATORY

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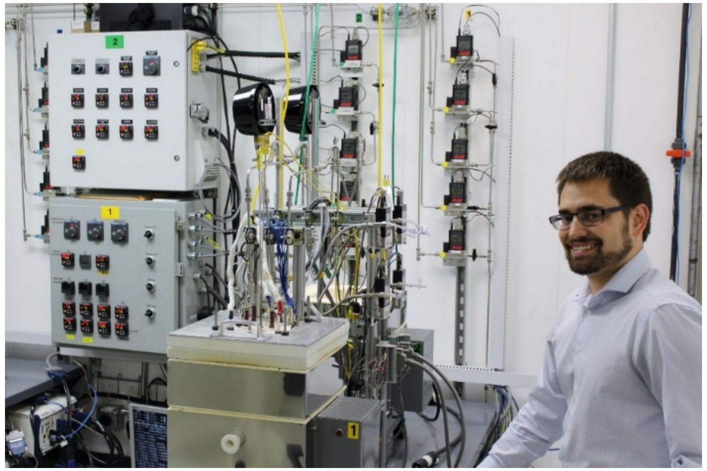

Questions

List of MOXIE Publications (1 of 2)

Thesis available at
www.forrestmeyen.com/publications

- Meyen, F., Krishnamurthy, A., Hoffman, J. A. "STPA Analysis of the Mars Oxygen Insitu Resource Utilization Experiment (MOXIE)" 2018 IEEE Aerospace Conference. Big Sky, Montana.
- Nasr, M., Meyen F., Hoffman, J.A. "Scaling the Mars Oxygen ISRU Experiment (MOXIE) for Mars Sample Return" 2018 IEEE Aerospace Conference. Big Sky, Montana.
- Meyen, F. "System Modeling, Design, and Control of the Mars Oxygen In-Situ Resource Utilization Experiment (MOXIE) and Implications for Atmospheric ISRU Processing Plants" Doctor of Philosophy Thesis. Massachusetts Institute of Technology Department of Aeronautics and Astronautics. May, 2017.
- Hartvigsen, J., Elangovan, S., Elwell, J., & Larsen, D. (2017). Oxygen Production from Mars Atmosphere Carbon Dioxide Using Solid Oxide Electrolysis. ECS Transactions, 78(1), 2953-2963.
- McClean, J. B., & Pike, W. T. (2017, June). Estimation of the Saltated Particle Flux at the Mars 2020 In-Situ Resource Utilization Experiment (MOXIE) Inlet. In Dust in the Atmosphere of Mars and Its Impact on Human Exploration (Vol. 1966).
- McClean, J. B., Merrison, J. P., Iversen, J. J., Madsen, M. B., Araghi, K., Meyen, F., ... & Voecks, G. (2017, March). Testing the Mars 2020 Oxygen In-Situ Resource Utilization Experiment (MOXIE) HEPA Filter and Scroll Pump in Simulated Mars Conditions. In Lunar and Planetary Science Conference (Vol. 48)

List of MOXIE Publications (2 of 2)

- Hecht, M. H., Hoffman, J. A., & Team, M. (2016, October). The Mars Oxygen ISRU Experiment (MOXIE) on the Mars 2020 Rover. In 3rd International Workshop on Instrumentation for Planetary Mission (Vol. 1980).
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- Hecht, M. H., Hoffman, J., Rapp, D., Voecks, G., Lackner, K. S., Hartvigsen, J., ... & De La Torre Juarez, M. (2014, December). The Mars Oxygen ISRU Experiment (MOXIE) on the yet-to-be-named Mars 2020 Lander. In AGU Fall Meeting Abstracts.

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- Meyen, F. "System Modeling, Design, and Control of the Mars Oxygen In-Situ Resource Utilization Experiment (MOXIE) and Implications for Atmospheric ISRU Processing Plants" Doctor of Philosophy Thesis. Massachusetts Institute of Technology Department of Aeronautics and Astronautics. May, 2017.
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Backup

Characterization Activities

1. SOXE stack performance dependence on operational parameters (I, V, P, T, m)
   a. Current voltage relationship
   b. Performance impacts at different cathode/anode pressures
   c. ASR Temperature dependence (General considerations see #4)
   d. Mass flow rate effects

2. Transient oscillation effects
   a. Pressure oscillation characterization (see flow C&C)
      - Effect of pressure oscillations on stack performance
   b. Characterize power supply oscillations
      - Effect of power supply oscillations on stack performance and degradation

3. SOXE stack degradation and lifetime (and resulting models)
   a. Stack degradation due to startup and shutdown operations (# of cycles)
   b. Long term stack degradation at constant operating conditions
   c. Long term stack degradation due to operation at elevated temperature.
   d. How to anticipate and avoid SOXE degradation
   e. Response to detected degradation
   f. Stack recovery potential after degradation
   g. Dynamic degradation near limits of coking
   h. Dynamic stack degradation near limits of oxidation
   i. Allowable operation before irreversible damage occurs
   j. Advanced remedies for carbon formation, oxidation, and/or perovskite oxygen loss (if any)

Characterization Activities

4. SOXE thermal characterization
    - a. Temperature distribution between cells for all operational states
        - Relationships to extrapolate between temperature sensors on the flight unit and fully instrumented stack
    - b. Thermal leakage and the relationship between heat provided to stack, heat leak, and O2 production
5. Voltage uncertainty
    - a. Amount of voltage loss over the leads to the SOXE
    - b. The importance of voltage uncertainty matter in current-controlled system if ASR is known
    - c. The effects of voltage gain error in the error measurement of ASR
    - d. Safe voltage operating limits
6. Cell-cell performance variation trends
    - a. Variation in CCASR at high flow vs low flow rates
    - b. Variation on measured voltages across flow rates
7. Sensor error, accuracy, and expected drift (to be provided by Sensor C&C)
    - a. Voltage
    - b. Current
    - c. Temperature
    - d. Flow meter
    - e. Pressure sensors

Characterization Activities

8. SOXE control system characterization
    a. Control authority and characteristics of our control system (ability to control V, T, P, Flow)
    b. Determination of optimal startup and shutdown sequences to minimize degradation risks, including stepwise profile
    c. Voltage based feedforward control (open loop)
    d. Cascaded current feedback control
    e. Safe Margin Active Reduction Tracking

9. Characterize the effect of flight instrumentation limitations on safe MOXIE operational command envelope

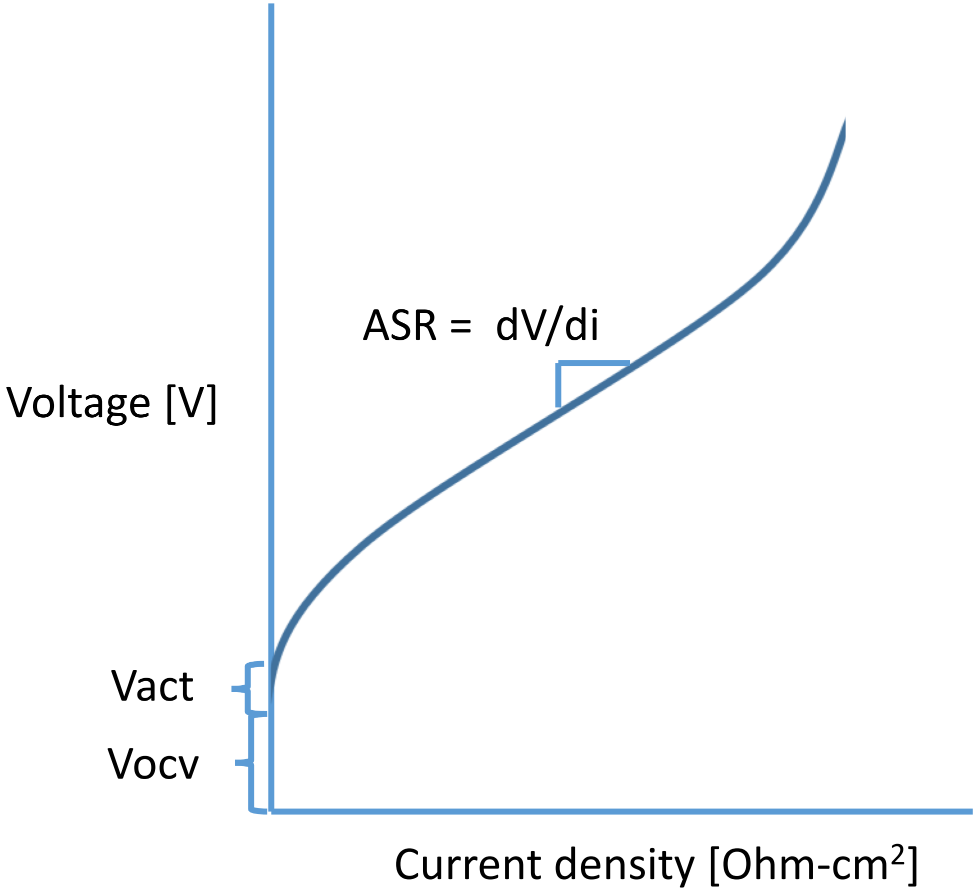
10. Fault detection isolation and recovery (FDIR)
    a. Crossover gas leak identification and quantification
    b. Electrical leak/short check at all phases
    c. Efficacy of hydrogen regeneration of cathode after testing for flight model

11. Expected behavior differences in SOXE performance and safe operational limits between test setups
    - Includes changes in system components (pump vs mass controller) and testing of electronics and control systems.

    a. Ceramatec vs. MDTB (JPL)
    b. MDTB vs. EM
    c. EM vs. Flight
    d. Flight vs. ATLO
    e. ATLO vs. surface operations

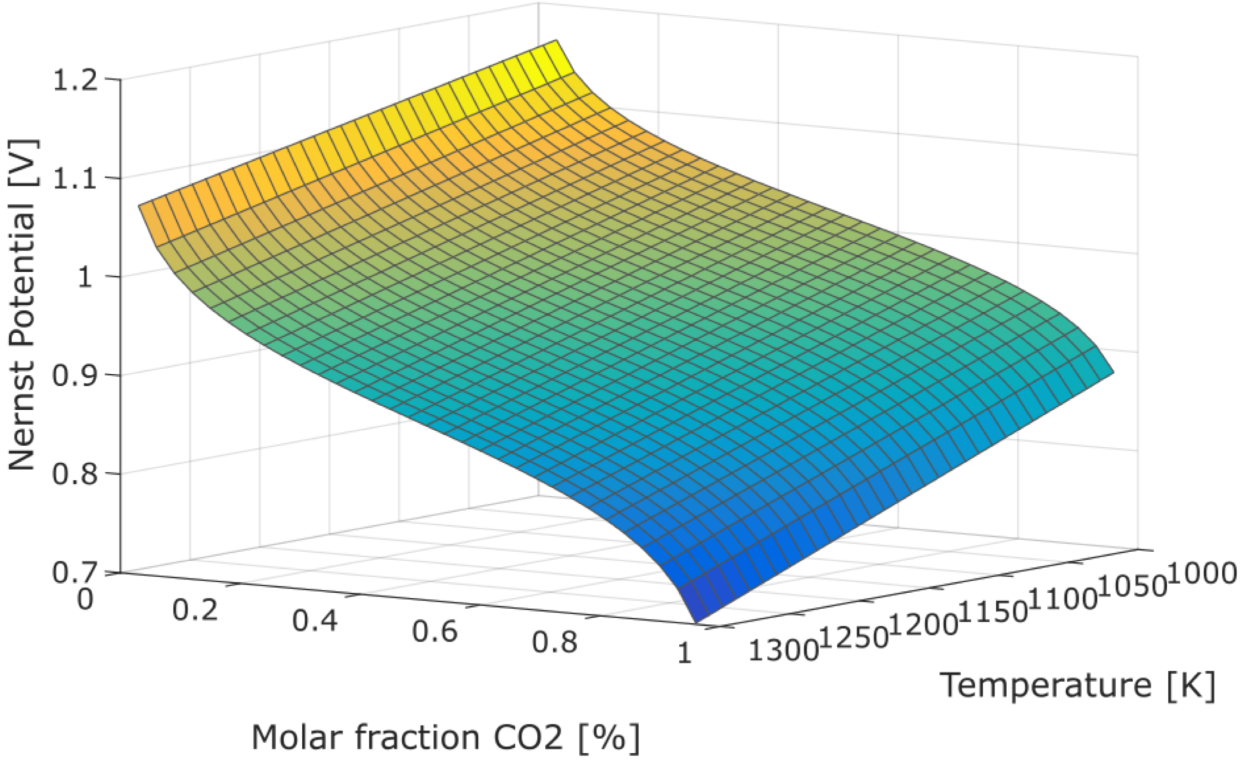
Area Specific Resistance

- Area specific resistance (ASR) is a key performance metric
- Units of Ohm-cm^2
- ASR is the slope of the current density and voltage relationship
- Represents cell performance
- Used to simplify model of the linear part of the i-V curve



Open circuit voltage and Nernst potential

- Open circuit voltage (Nernst potential at stack inlet)
- $V_{ocv} = V_{rev} + \frac{RT}{4F} ln\left[\frac{(P_{CO}^0)^2 P_{O_2}^0}{(P_{CO_2}^0)^2}\right]$
- Reversible voltage
- $V_{rev} = \frac{-\Delta G_f^\circ}{4F}$
- Linear approximation for V_{rev}
- $V_{rev} = -4.492 * 10^{-4}(T) + 1.462$



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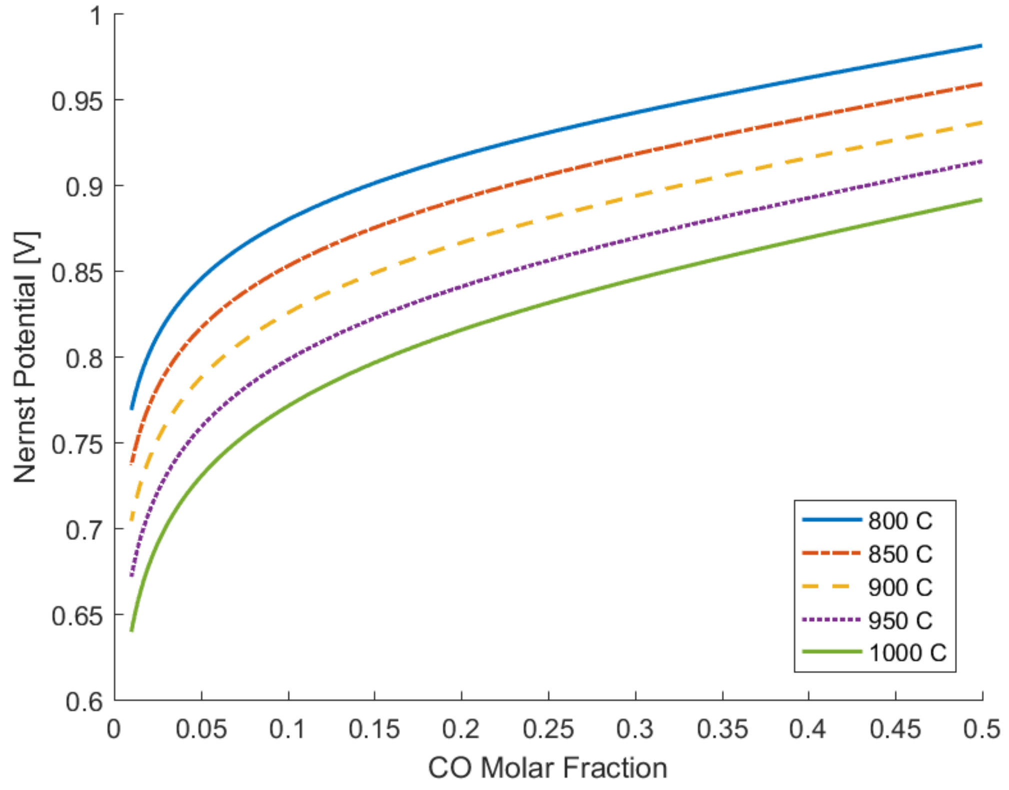
Average Nernst potential across SOXE stack



Improving 1D estimate of V_{Nernst}

$$V_{Nernst,Ave} = \frac{1}{x_{co,out} - x_{co,in}} \int_{x_{co.in}}^{x_{co,out}} \left(E_0 + \frac{RT}{4F} ln \left[\frac{(P_c * x_{co})^2 P_{O_2}^0}{(P_c * (1 - x_{co}))^2} \right] \right) dx_{co}$$

Other important equations

- Thermal neutral voltage

$$V_{tn} = \frac{\Delta H_f}{4F} \qquad V_{tn} = -8.655(10^{-9})T^2 - 1.496(10^{-6})T + 1.475$$

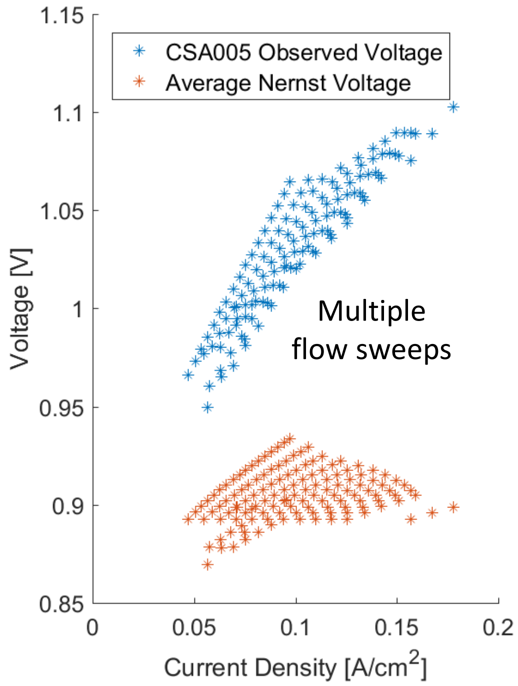
$$\dot{Q}_{gen} = I(V_{op} - V_{tn})$$

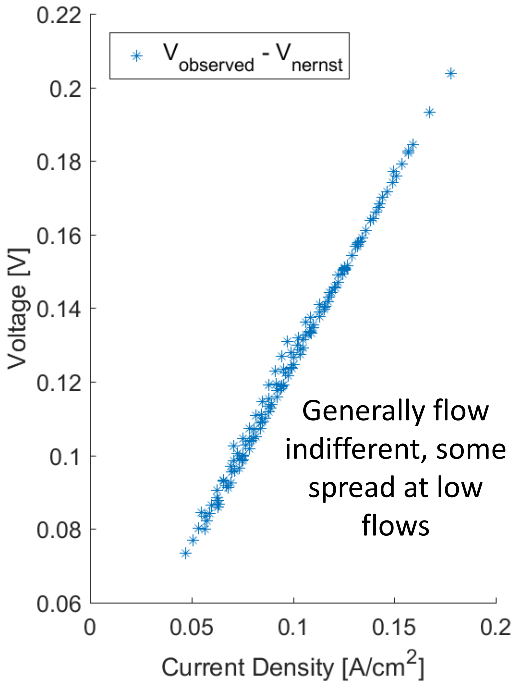
Meyen 2015

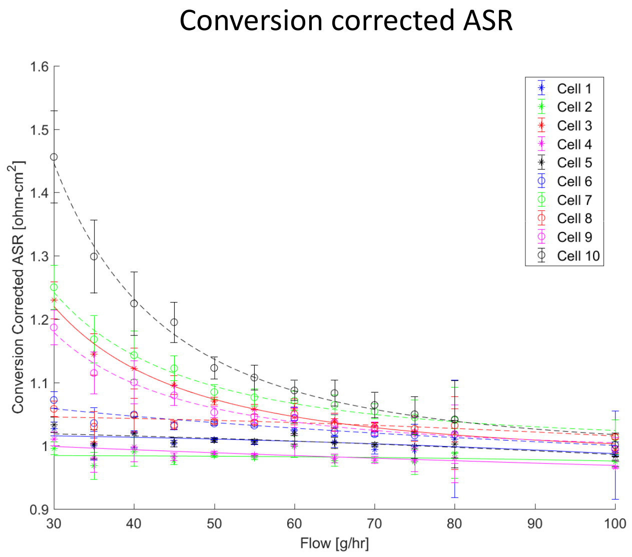
Model Development

$$V_{conv.correct} = V_{observed} - V_{Nernst,ave}$$

$$V_{Nernst,Ave} = \frac{1}{x_{co,out} - x_{co,in}} * \left[\frac{-\Delta G_f^o}{4F} x_{co} + \frac{RT}{4F}\left(x_{co} \ln\left(\frac{P_{O_2} * x_{co}^2}{(x_{co} - 1)^2}\right) + 2\ln(1 - x_{co})\right)\right]_{x_{co,in}}^{x_{co,out}}$$







Conversion corrected ASR is the slope the remaining i-V relationship

Meyen Thesis 2017