Modeling Electrolytic Conversion of Metabolic CO_2 and Optimizing a Microfluidic Electrochemical Reactor for Advanced Closed Loop Life Support Systems

236th ECS Meeting, Atlanta, GA Oct. 13-17 2019

National Aeronautics and Space Administration

Jesus Dominguez (IG/JSEG), Brittany Brown (NASA),
Brian Dennis (UTA), Wilaiwan Chanmanee (UTA),
Peter Curreri (NASA)

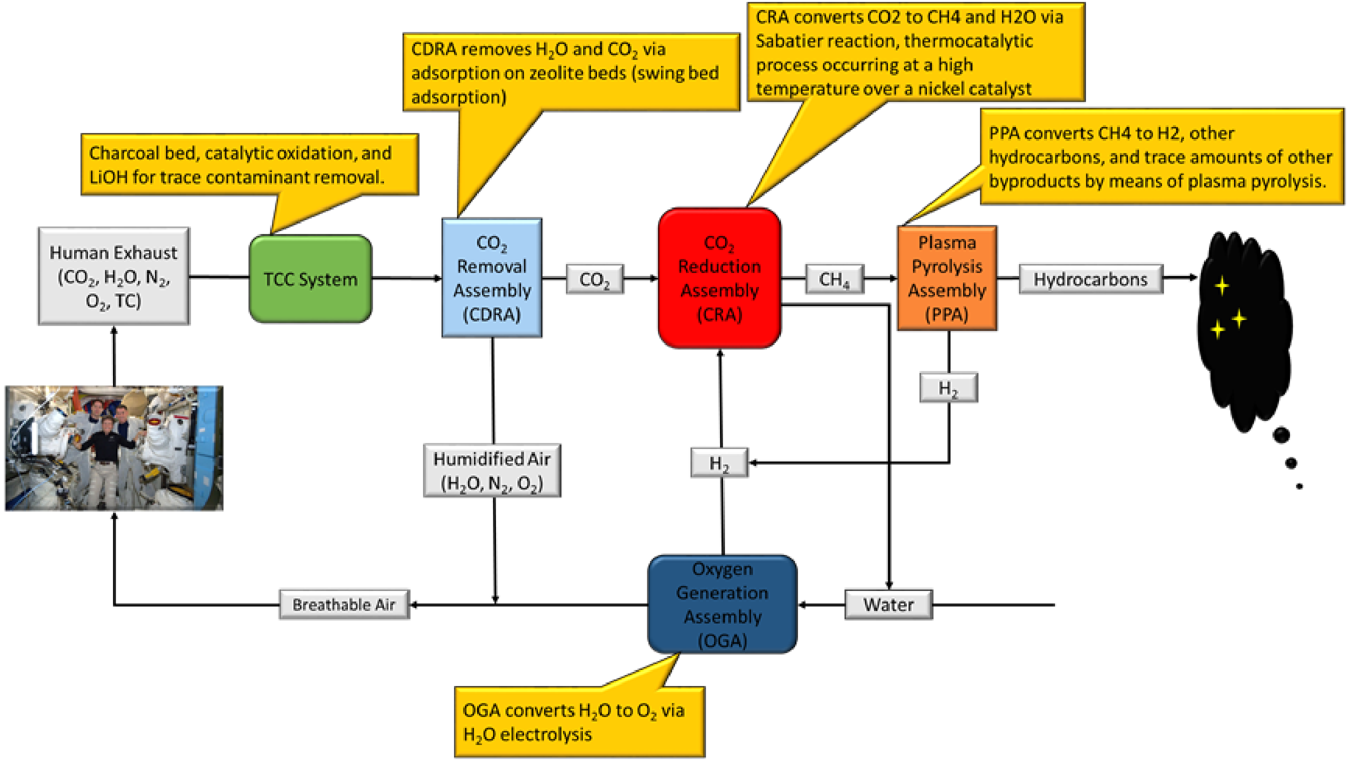
IG	: Insight Global
JSEG	: Jacobs Space Exploration Group
UTA	: University of Texas in Arlington
NASA	: National Aeronautics and Space Administration

MARSHALL
SPACE FLIGHT CENTER

Current Exploration O_2 Recovery System Baseline

Current O_2 Recovery: ~50%

☐ Extremely high temperatures result in heavy reactors and high power consumption



Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

CDRA removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption)

CRA converts CO2 to CH4 and H2O via Sabatier reaction, thermocatalytic process occurring at a high temperature over a nickel catalyst

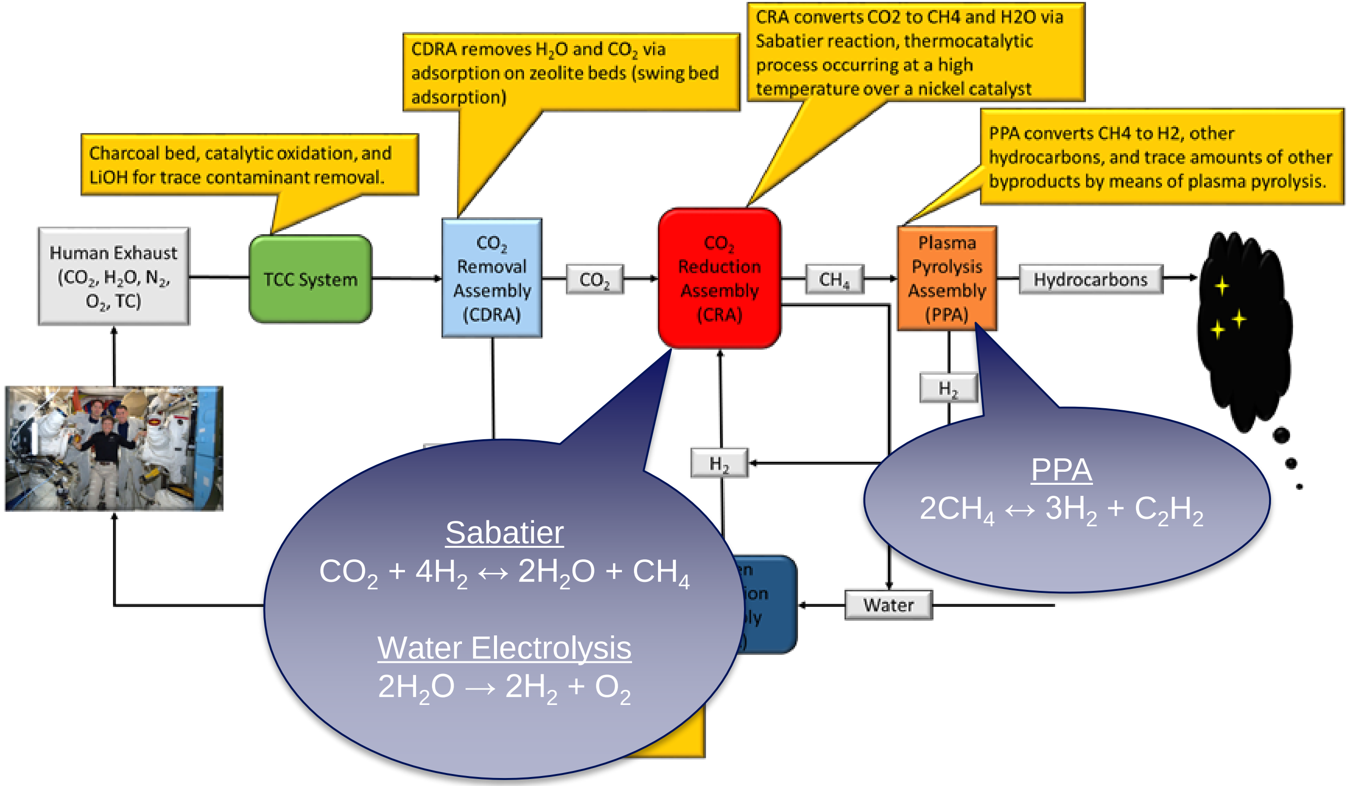
PPA converts CH4 to H2, other hydrocarbons, and trace amounts of other byproducts by means of plasma pyrolysis.

OGA converts H_2O to O_2 via H_2O electrolysis

Current Exploration O_2 Recovery System Baseline

Current O_2 Recovery: ~50%

- ☐ Extremely high temperatures result in heavy reactors and high power consumption



Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

CDRA removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption)

CRA converts CO2 to CH4 and H2O via Sabatier reaction, thermocatalytic process occurring at a high temperature over a nickel catalyst

PPA converts CH4 to H2, other hydrocarbons, and trace amounts of other byproducts by means of plasma pyrolysis.

Human Exhaust (CO_2, H_2O, N_2, O_2, TC)

TCC System

CO_2 Removal Assembly (CDRA)

CO_2

CO_2 Reduction Assembly (CRA)

CH_4

Plasma Pyrolysis Assembly (PPA)

Hydrocarbons

H_2

H_2

Water

Sabatier

$CO_2 + 4H_2 \leftrightarrow 2H_2O + CH_4$

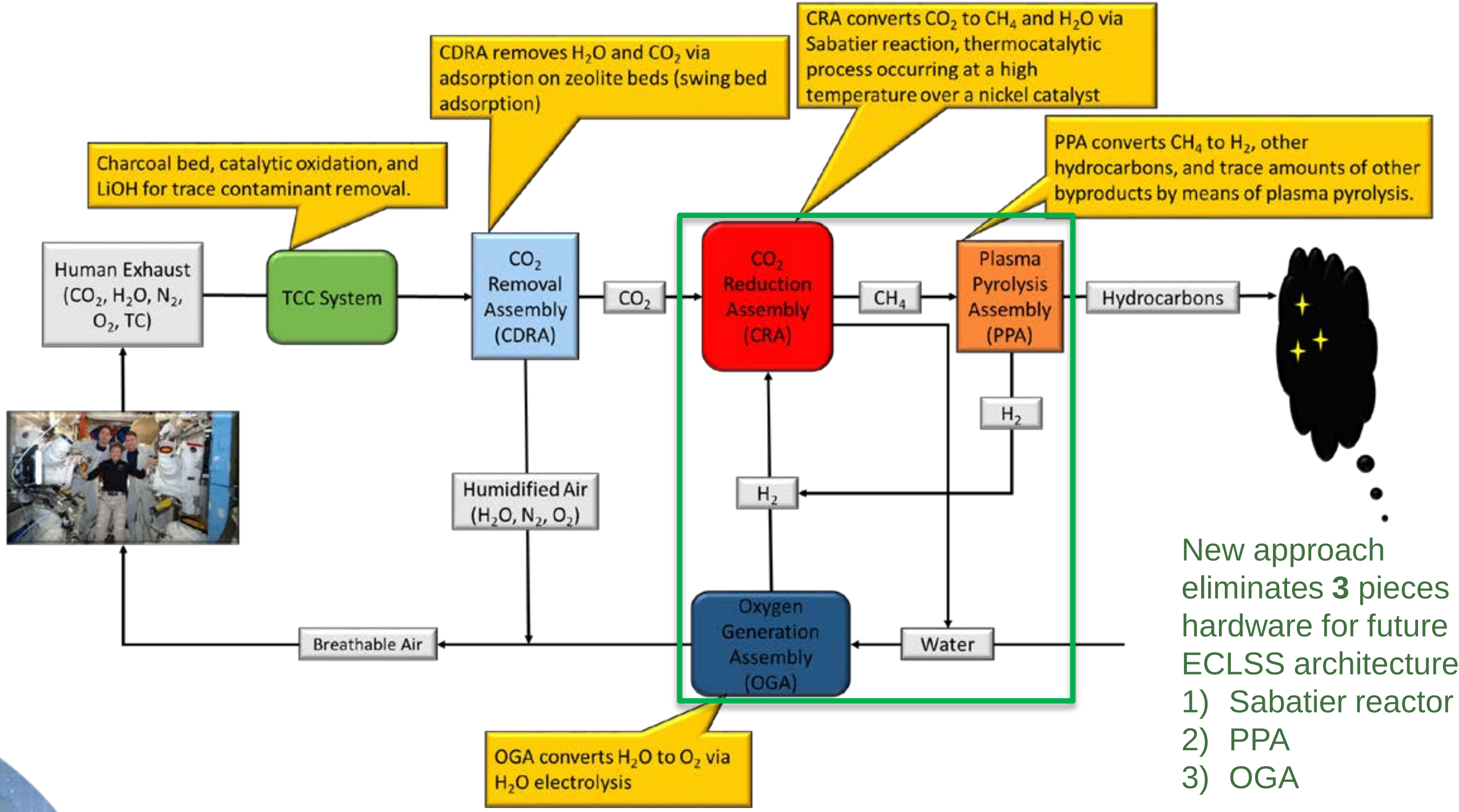
Water Electrolysis

$2H_2O \rightarrow 2H_2 + O_2$

PPA

$2CH_4 \leftrightarrow 3H_2 + C_2H_2$

Advanced O_2 Recovery System via Electrolytic Technology



Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

CDRA removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption)

CRA converts CO_2 to CH_4 and H_2O via Sabatier reaction, thermocatalytic process occurring at a high temperature over a nickel catalyst

PPA converts CH_4 to H_2, other hydrocarbons, and trace amounts of other byproducts by means of plasma pyrolysis.

OGA converts H_2O to O_2 via H_2O electrolysis

Human Exhaust (CO_2, H_2O, N_2, O_2, TC)

TCC System

CO_2 Removal Assembly (CDRA)

CO_2

CO_2 Reduction Assembly (CRA)

CH_4

Plasma Pyrolysis Assembly (PPA)

Hydrocarbons

H_2

H_2

Humidified Air (H_2O, N_2, O_2)

Oxygen Generation Assembly (OGA)

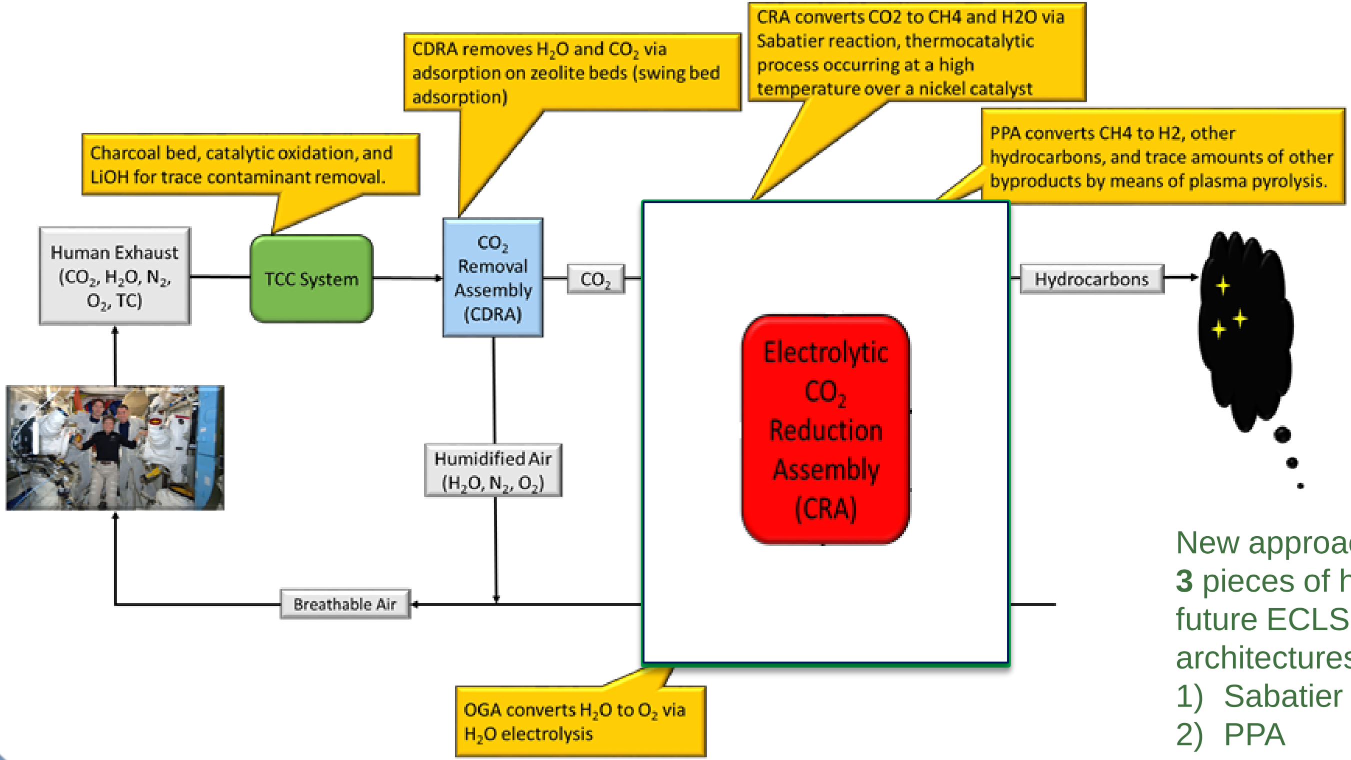
Water

Breathable Air

New approach eliminates **3** pieces of hardware for future ECLSS architectures:

1) Sabatier reactor
2) PPA
3) OGA

Advanced O_2 Recovery System via Electrolytic Technology



Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

$CDRA$ removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption)

CRA converts CO2 to CH4 and H2O via Sabatier reaction, thermocatalytic process occurring at a high temperature over a nickel catalyst

PPA converts CH4 to H2, other hydrocarbons, and trace amounts of other byproducts by means of plasma pyrolysis.

Human Exhaust (CO_2, H_2O, N_2, O_2, TC)

TCC System

CO_2 Removal Assembly (CDRA)

CO_2

Electrolytic CO_2 Reduction Assembly (CRA)

Hydrocarbons

Humidified Air (H_2O, N_2, O_2)

Breathable Air

OGA converts H_2O to O_2 via H_2O electrolysis

New approach eliminates **3** pieces of hardware for future ECLSS architectures:

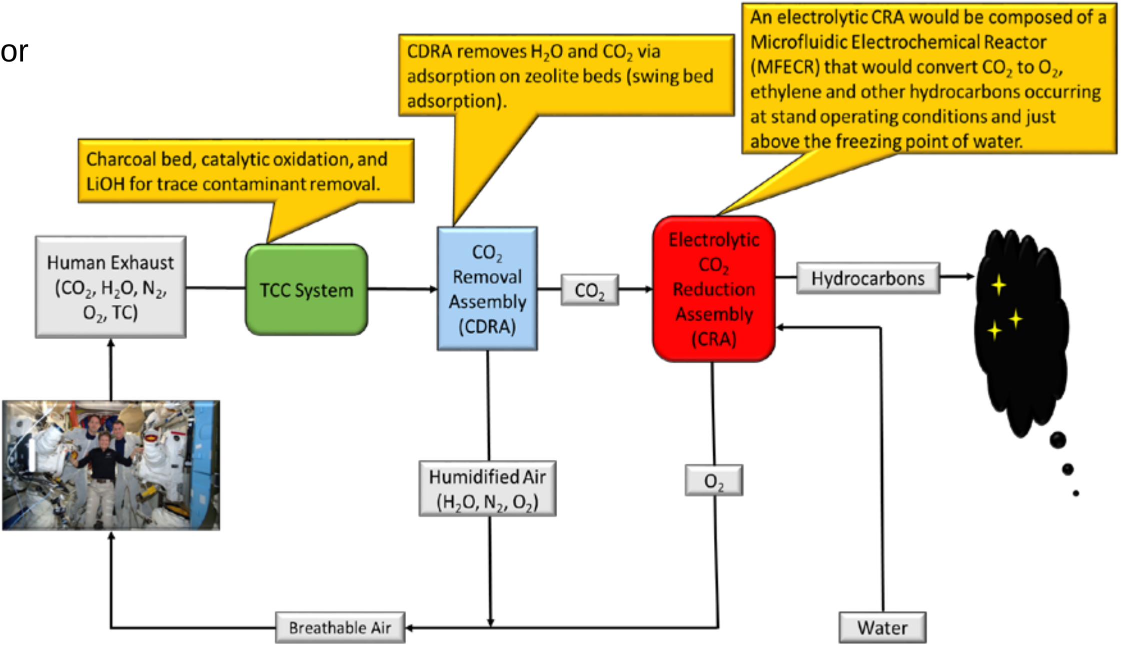
1) Sabatier reactor
2) PPA
3) OGA

Advanced O_2 Recovery System via Electrolytic Technology

Eliminates **3** pieces of hardware for future ECLSS architectures:

1) Sabatier reactor
2) PPA
3) OGA

- Higher O_2 recovery rate
- Higher reliability
- Less complex
- Lower power consumption
- Lower mass


Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

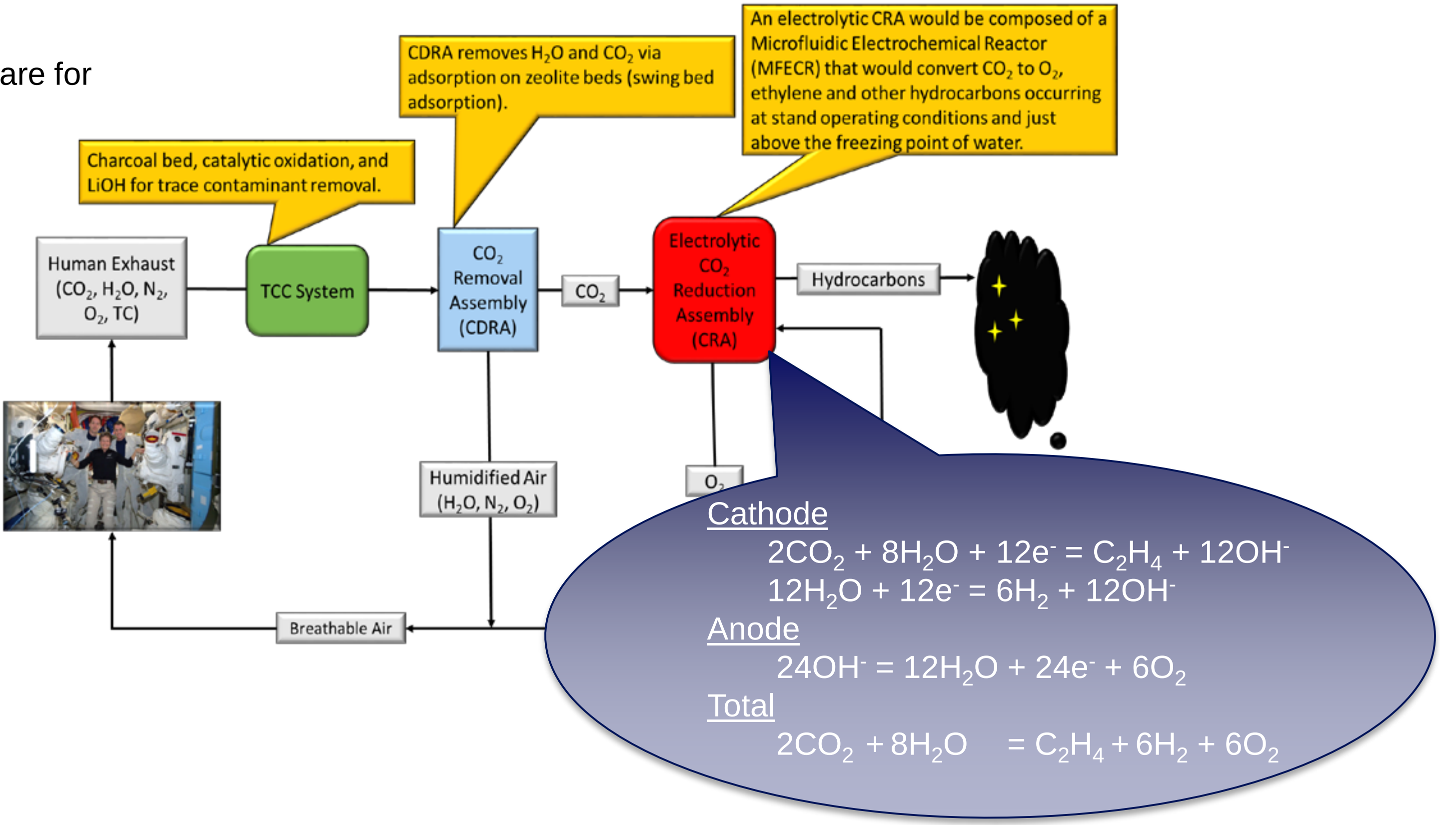
CDRA removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption).

An electrolytic CRA would be composed of a Microfluidic Electrochemical Reactor (MFECR) that would convert CO_2 to O_2, ethylene and other hydrocarbons occurring at stand operating conditions and just above the freezing point of water.

Eliminates **3** pieces of hardware for future ECLSS architectures:

1) Sabatier reactor
2) PPA
3) OGA

- Higher O_2 recovery rate
- Higher reliability
- Less complex
- Lower power consumption
- Lower mass



Charcoal bed, catalytic oxidation, and LiOH for trace contaminant removal.

CDRA removes H_2O and CO_2 via adsorption on zeolite beds (swing bed adsorption).

An electrolytic CRA would be composed of a Microfluidic Electrochemical Reactor (MFECR) that would convert CO_2 to O_2, ethylene and other hydrocarbons occurring at stand operating conditions and just above the freezing point of water.

Cathode

$2CO_2 + 8H_2O + 12e^- = C_2H_4 + 12OH^-$

$12H_2O + 12e^- = 6H_2 + 12OH^-$

Anode

$24OH^- = 12H_2O + 24e^- + 6O_2$

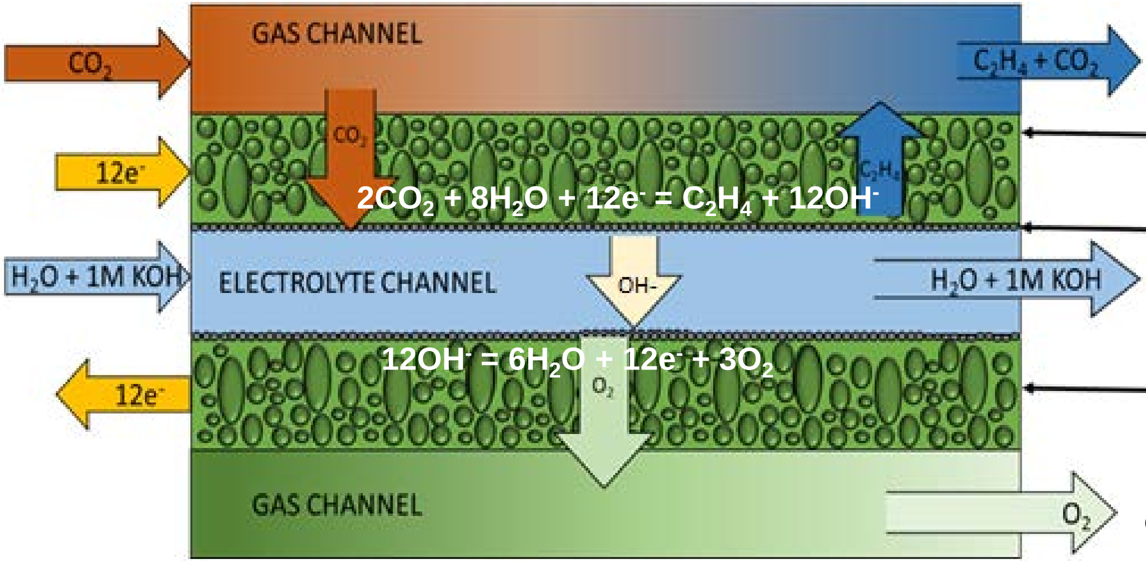
Total

$2CO_2 + 8H_2O = C_2H_4 + 6H_2 + 6O_2$

Advanced O_2 Recovery System via Electrolytic Technology

Development of Advanced O_2 Electrolytic Recovery System

In 2016, NASA's Game Changing Development Program awarded the University of Texas at Arlington to develop a microfluidic electrochemical reactor (MFECR) to convert CO_2 into oxygen and ethylene with a theoretical oxygen recovery rate of 73%.



$2CO_2 + 8H_2O + 12e^- = C_2H_4 + 12OH^-$

$12OH^- = 6H_2O + 12e^- + 3O_2$

OH⁻

- ☐ H_2O occasionally added from WPA
- ☐ KOH is not consumed
- ☐ GDL electrodeposited layer of nano-particles (patented by UTA)

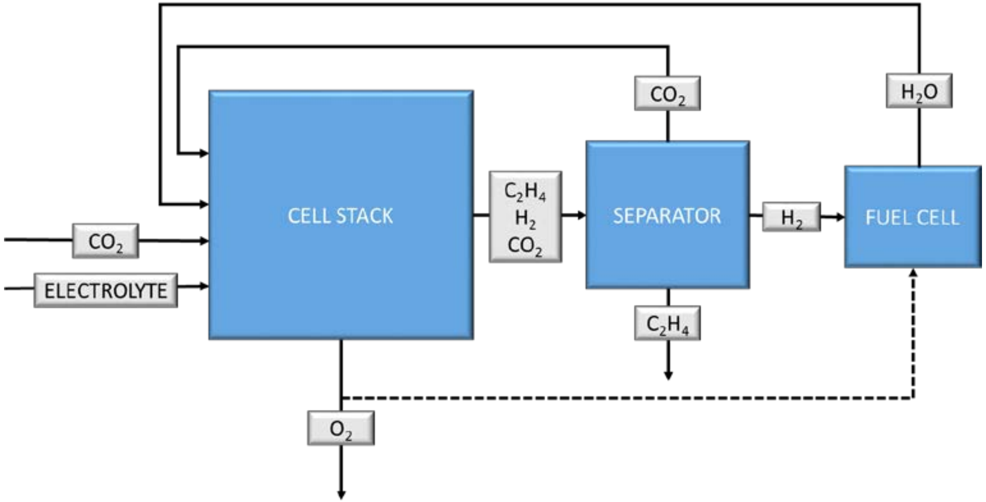
Theoretical O_2 Recovery Rate: **73%**

Technology Advancement Overview

ENGINEERING + UNIVERSITY OF TEXAS ARLINGTON INNOVATIVE CHEMISTRY = GAME CHANGING ELECTROCHEMICAL REACTOR FOR ADVANCED ECLSS

PROJECT OBJECTIVES

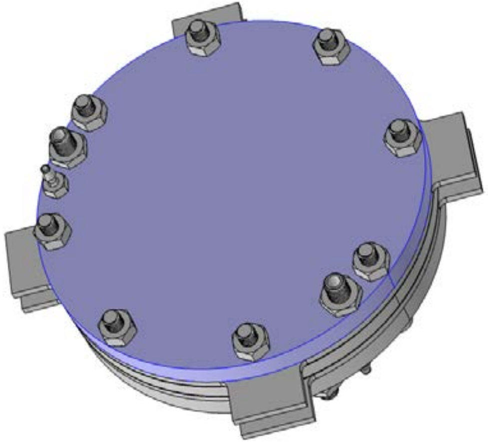
1. Advance the technology readiness of the proposed technology to TRL 4.
2. To increase the O_2 recovery efficiency of the process to >50% (from 37% currently)
3. To mature the hardware system to process 1.0 kg/day of CO_2



MFECR’s 3D Model

- 3D Multi-physics model developed at NASA Marshall Space Flight Center (MFSC) on electrochemical CO_2 conversion to O_2 and C_2H_4 at ambient conditions via MFECR.
- In the model the electrochemical physics is coupled with all the other physics phenomena involved in the process, such as fluid flow and mass transfer of reactant/product species in free and porous media, convective/conduction/radiative heat transfer, as well as conduction of DC electrical current with Joule heating generation.
- This work aims to use this 3D model to build a comprehensive, rigorous, and experimentally validated simulator that will be used as a valuable tool to not only assist the authors on the EDU design but also to optimize its operation.

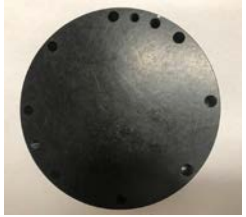
Fabrication of MFECR’s elements (CAD’s drawings)



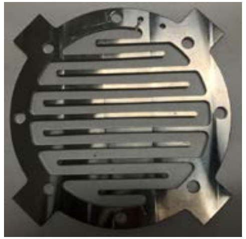
CAD drawing used to fabricate the MFECR’s elements as material domains for the model.

Assembled MFECR’s elements

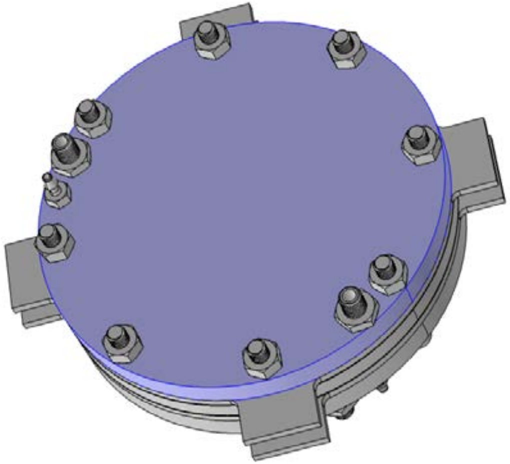
End plate



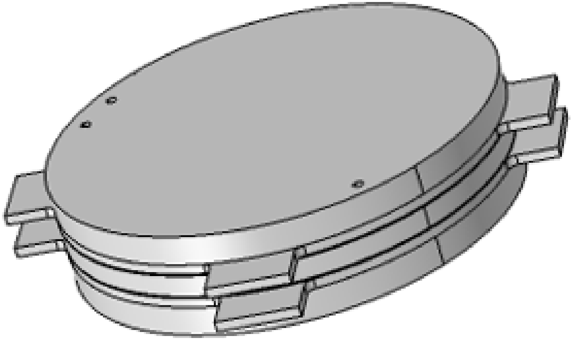
Electrode



Electrolyte wall



MFECR’s CAD drawing

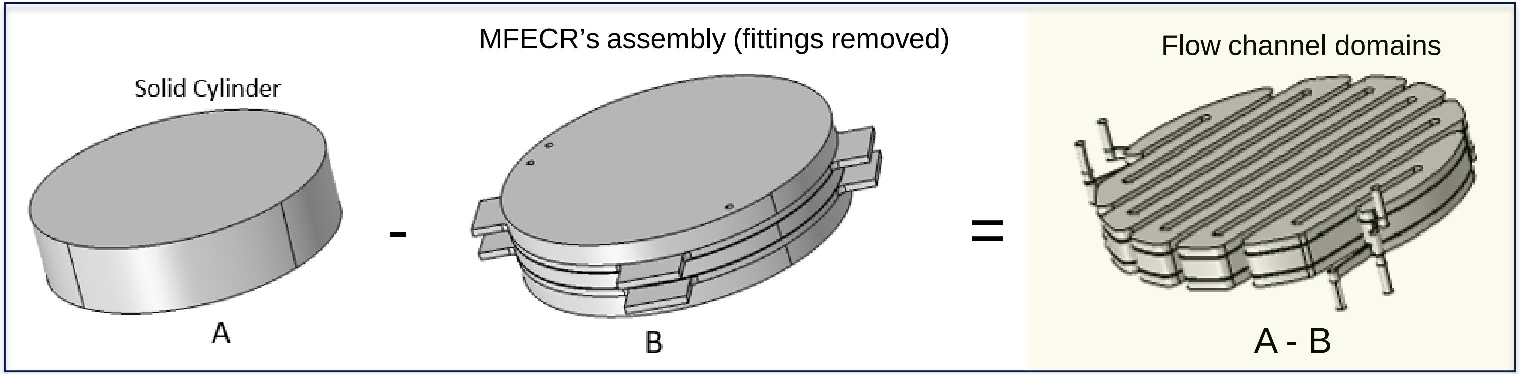


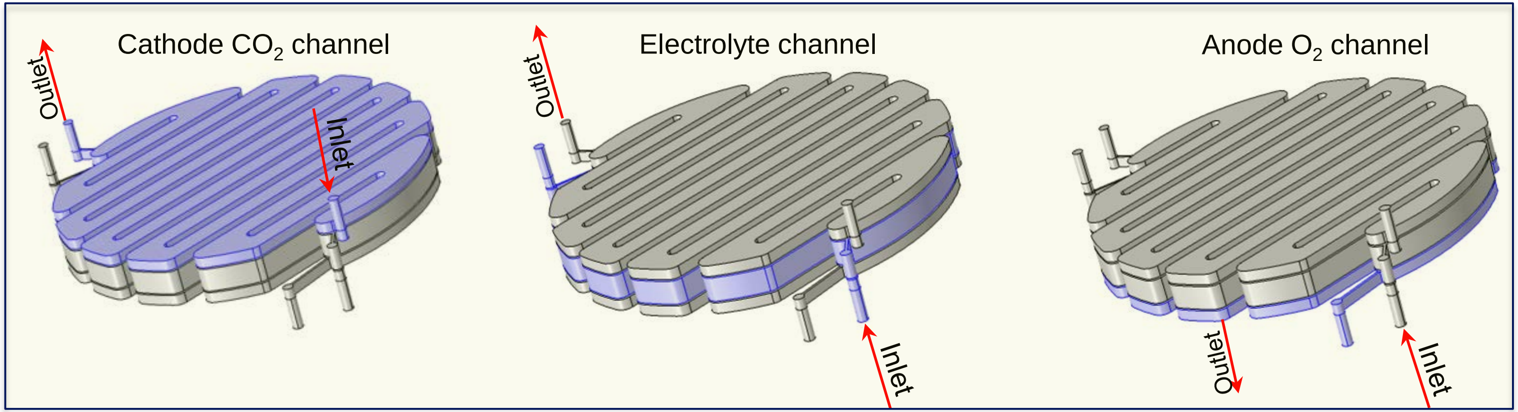
MFECR’s model domain (fittings removed)

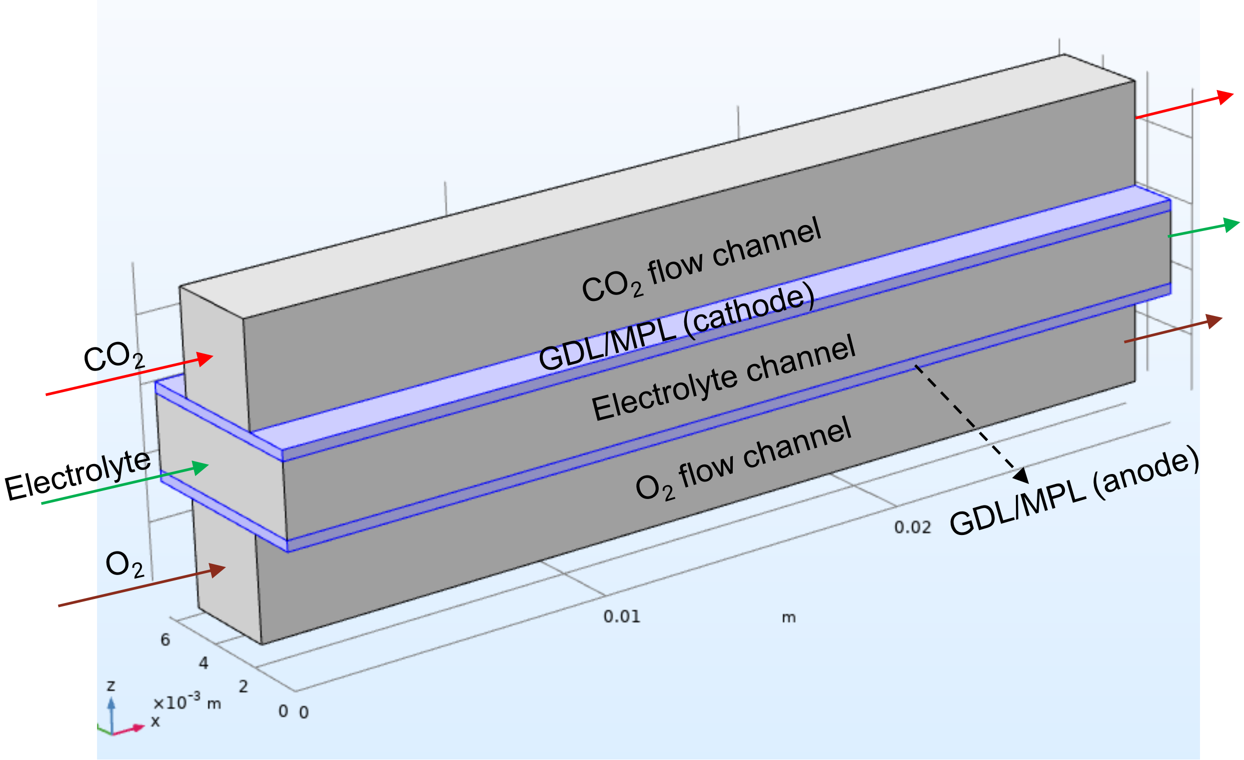
MFECR model’s memory required**:** 185 GB
High-Performance Computer (512 GB RAM)**:**
Physical memory 183 GB
Virtual memory 2 GB

MFECR model’s material domains

MFECR Model’s flow domains





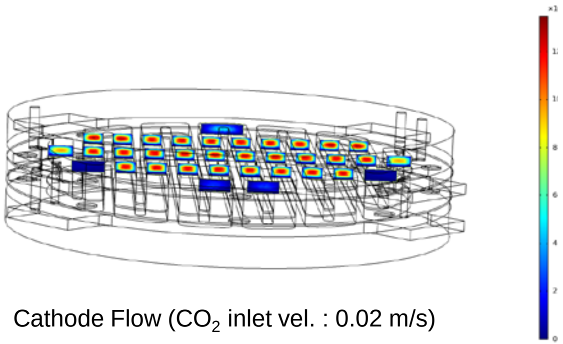


MFECR's Straight Section

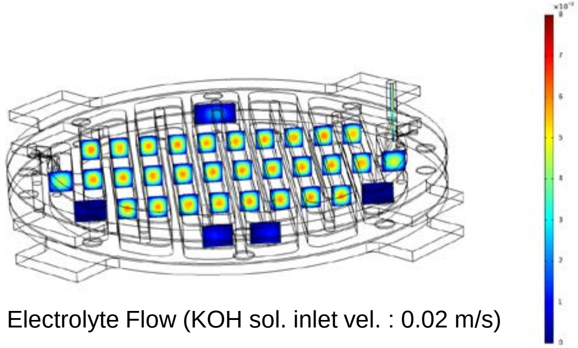
Model's Flow Domains

Model approach on flow rate and pressure

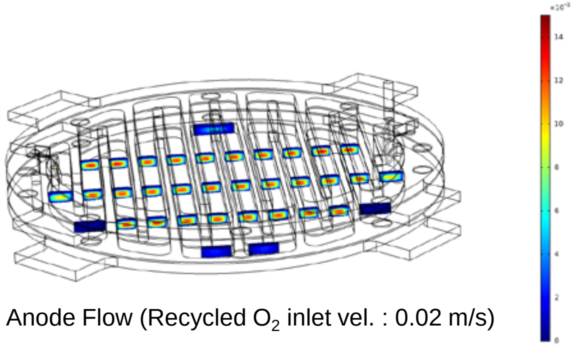
Free Flow Rate and Pressure on Serpentines (cathode, electrolyte, and anode)



Cathode Flow (CO_2 inlet vel. : 0.02 m/s)

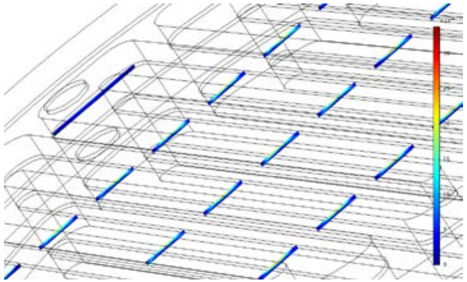


Electrolyte Flow (KOH sol. inlet vel. : 0.02 m/s)



Anode Flow (Recycled O_2 inlet vel. : 0.02 m/s)

Porous Flow Rate and Pressure on GDLs (cathode and anode)



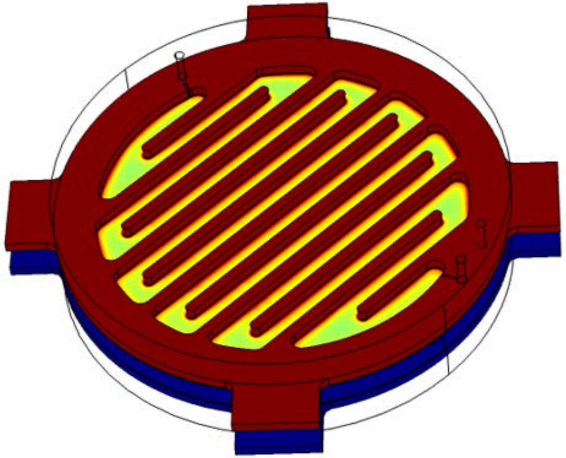
Cathode Flow (CO_2 inlet vel. : 0.02 m/s)

Brinkman approach for velocity/pressure:

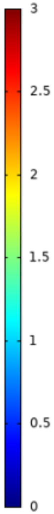
- free medium on serpentines
- porous medium on GDL and MPL.

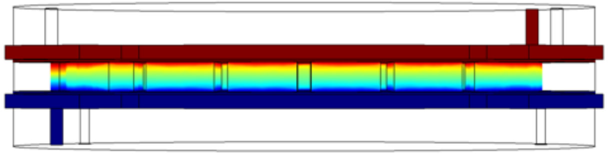
Maxwell-Stefan approach for mass transport of concentrated species on serpentines, GDL, and MPL.

Model approach on DC current generation



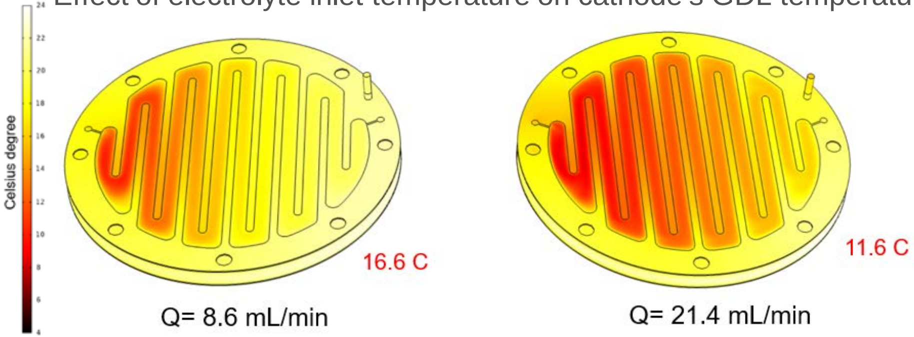
Electrical potential applied : 3V

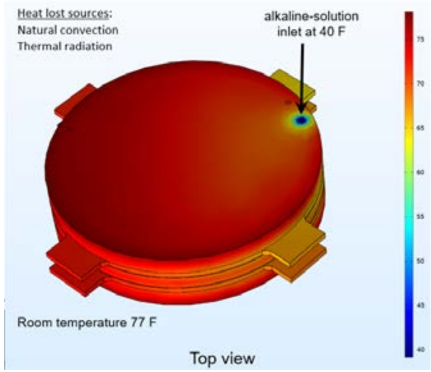


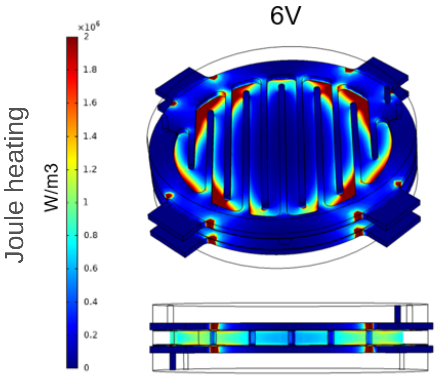


Given a differential electrical potential applied between electrodes, Ohm's law and the charge conservation equation is used to determine current/potential distribution through all MFECR’s elements.

Effect of electrolyte inlet temperature on cathode’s GDL temperature







Heat transfer mechanisms:

- Conduction
- Free convection outer surface – ambient
- Thermal radiation outer surface – ambient
- Flowing gas/liquid convection
- Joule heating

Model approach on heat transfer

Model’s Electrochemical reactions on GDL domains

CO_2 Conversion to C_2H_4 with H_2 as byproduct

Acid Electrolyte	**E^o (V)**
Cathode	
$2CO_2 + 12H^+ + 12e^- = C_2H_4 + 4H_2O$	-0.35
$12H^+ + 12e^- = 6H_2$	0.00
Anode	
$12H_2O = 24H^+ + 24e^- + 6O_2$	-1.23
Total	
$2CO_2 + 8H_2O = C_2H_4 + 6H_2 + 6O_2$	-1.58

Alkaline Electrolyte	
Cathode	
$2CO_2 + 8H_2O + 12e^- = C_2H_4 + 12OH^-$	-1.18
$12H_2O + 12e^- = 6H_2 + 12OH^-$	-0.40
Anode	
$12OH^- = 6H_2O + 12e^- + 3O_2$	-0.83
Total	
$2CO_2 + 8H_2O = C_2H_4 + 6H_2 + 6O_2$	-2.41

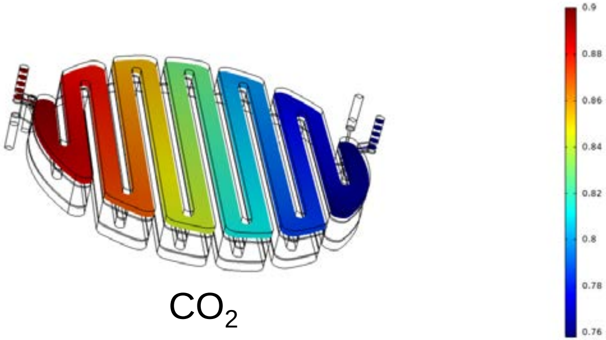
H_2O Electrolysis

Acid Electrolyte	**E^o (V)**
Cathode	
$4H^+ + 4e^- = 2H_2$	0.00
Anode	
$2H_2O = 4H^+ + 4e^- + O_2$	-1.23
Total	
$2H_2O = 2H_2 + O_2$	-1.23

Alkaline Electrolyte	
Cathode	
$4H_2O + 4e^- = 2H_2 + 4OH^-$	-0.40
Anode	
$4OH^- = 2H_2O + 4e^- + O_2$	-0.83
Total	
$2H_2O = 2H_2 + O_2$	-1.23

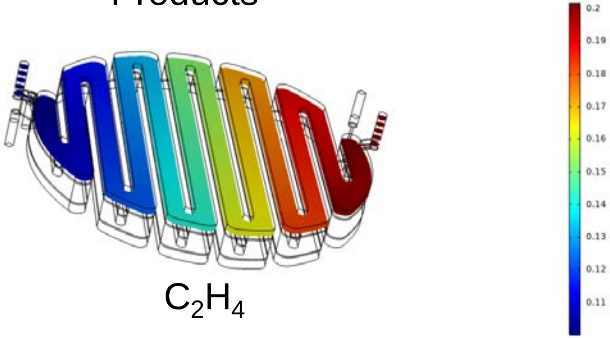
Model approach on EC cathodic reactions

Reactant

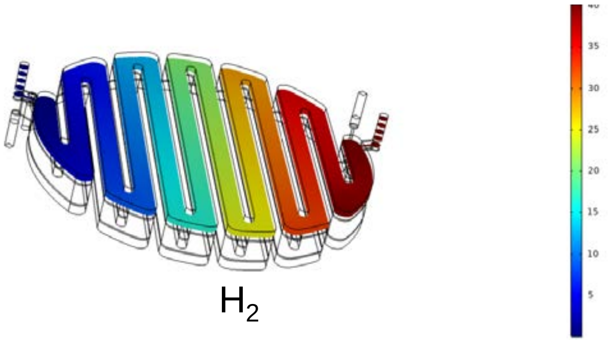


CO_2

Products



C_2H_4



H_2

Conclusions

- A rigorous model has been developed and deployed to simulate a MFECR unit and optimize the design and performance.
- The MFECR unit is equipped with the instrumentation and meters that will allow full validation of the model including determination of the electrochemical kinetics parameters.