ISRU SYSTEM MODEL TOOL: FROM EXCAVATION TO OXYGEN PRODUCTION. E. Santiago-Maldonado¹ and D. L. Linne², ¹NASA KSC Mail Code KT-D Kennedy Space Center, FL 32828, Edgardo.Santiago-Maldonado-1(nasa.gov, ²NASA GRC, MS 301-3 21000 Brookpark Rd Cleveland, OH 44135, Diane.L.Linne@nasa.gov

Introduction:
In the late 80's, conceptual designs for an in situ oxygen production plant were documented in a study by Eagle Engineering [1]. In the “Summary of Findings” of this study, it is clearly pointed out that: “reported process mass and power estimates lack a consistent basis to allow comparison.” The study goes on to say: “A study to produce a set of process mass, power, and volume requirements on a consistent basis is recommended.” Today, approximately twenty years later, as humans plan to return to the moon and venture beyond, the need for flexible up-to-date models of the oxygen extraction/production process has become even more clear.

Multiple processes for the production of oxygen from lunar regolith are being investigated by NASA, academia, and industry. Three processes that have shown technical merit are molten regolith electrolysis, hydrogen reduction, and carbothermal reduction. These processes have been selected by NASA as the basis for the development of the ISRU System Model Tool (ISMT). In working to develop up-to-date system models for these processes NASA hopes to accomplish the following: (1) help in the evaluation process to select the most cost-effective and efficient process for further prototype development, (2) identify key parameters, (3) optimize the excavation and oxygen production processes, and (4) provide estimates on energy and power requirements, mass and volume of the system, oxygen production rate, mass of regolith required, mass of consumables, and other important parameters. Also, as confidence and high fidelity is achieved with each component’s model, new techniques and processes can be introduced and analyzed at a fraction of the cost of traditional hardware development and test approaches. A first generation ISRU System Model Tool has been used to provide inputs to the Lunar Architecture Team studies.

Model Description:
A typical end-to-end ISRU system model is composed of a regolith excavation system, regolith feed system, chemical processing plant, and liquefaction and storage system. The system model is divided into modules that represent unit operations (e.g., electrolyzer, gas separator, reactor, liquefaction, etc). This modularity (plug-n-play) feature allows the use of the same unit operation model in different oxygen production systems simulations, resulting in comparable and consistent results. Each unit operation is modeled theoretically using Excel and Visual Basic for Applications (VBA), and validated using available experimental data from on-going laboratory work. Each module contains a worksheet called “Databus” that functions as an interface between modules. This Databus contains input and output fields, where parameters are grouped into arrays using the Range Name feature of Excel. These arrays are m-by-1 matrices (m being the number of parameters in the array), and can include strings, booleans, and numerical values.

Modules are linked to each other using ‘flow arrays’ containing temperature, pressure, and flow rates of each compound present in the stream. Furthermore, each module contains “Global” Inputs/Outputs and “Design” Inputs/Outputs. Global I/O are those parameters of interest at the high level such as location of lunar outpost, type of power system, mass, power, volume, etc. Design I/O are those parameters that are specific to each module such as efficiency, diameter, materials, etc.

ISRU System Model Tool:
The ISMT consists of sub-systems integrated using a commercial off-the-shelf model integration software [2]. This software offers a graphical interface to link or connect each Excel model file, a trade study tool, a parametric study tool, and an optimization tool. The ISMT consists of: Excavation sub-system, Regolith Handling sub-system, Reactor sub-system, Electrolyzer sub-system, Liquefaction sub-system, and Thermal Energy sub-system. The following is a brief description of the capabilities and features of these sub-systems:

Excavation sub-system:
- Force module calculates forces on digging tools and wheels/tracks based on classical soil mechanics correlations; dimensions of digging tool, wheels, and chassis; and power/energy requirements for digging and driving operations.
- Mass module calculates the mass of individual components (digging tool, boom arm, motors & actuators, chassis, etc.) based on the dimensions and forces calculated in force module.
- Options for bucket wheel, front-end loader, backhoe, and bull-dozer blade.
- Options for wheels or tracks.
- Options for continuous or intermittent digging.
• Capability to vary vehicle velocity, depth of cut, soil properties, surface slope (for driving), digging rate (e.g., regolith per day), per-delivery load, down-time between deliveries, and many other variables.

Regolith Handling sub-system:
• Includes feed and dump hoppers and augers.
• Hoppers are sized based on amount of regolith stored.
• Augers have an option for heat exchange between the feed auger (cold regolith) and dump auger (hot-spent regolith).

Reactor sub-system:
• Options for carbothermal processing, hydrogen reduction processing, and molten regolith electrolysis.
• Carbothermal processing option includes a carbothermal reactor, desulfurization unit, and methanation reactor. Carbothermal reactor, desulfurization, and methanation reactor models are based on recent design concepts [3].
• Hydrogen reduction processing option includes a hydrogen reduction reactor and desulfurization unit. Hydrogen reduction reactor has options for a fluidized bed, loosely-packed bed, and a rotating bed (currently being developed) [4].

Electrolyzer sub-system:
• Options for proton exchange membrane (PEM) and solid oxide (SO) electrolyzer.
• PEM electrolyzer option includes a micro-channel heat exchanger, condenser, water pump, phase separator, PEM electrolyzer, and a water absorption bed.
• SO electrolyzer option includes gas phase separators and SO electrolyzer.

Liquefaction sub-system:
• The liquefaction sub-system includes radiators, cryocoolers, and storage tanks. This sub-system has an option for single or multiple cryocoolers for condensing the oxygen produced and managing boil-off.

Thermal Energy sub-system:
• The thermal energy sub-system includes a rigid solar concentrator [3] to provide thermal energy to the reactors. An inflatable solar concentrator option is currently being developed.

The latest version of the ISRU System Modeling Tool will be presented along with results and trade studies of various system configurations.

Acknowledgment:
This work is funded by the ISRU Project under the Exploration Technology Development Program (ETDP). Many thanks to the model development team at Glenn Research Center and Kennedy Space Center, without their hard work and dedication this work could not have been completed.

References:
ISRU System Model Tool: From Excavation to Oxygen Production

Edgardo Santiago-Maldonado - KSC
Diane L. Linne - GRC
ISRU System Model Tool

- **Capability:**
  - System optimization
  - Allows integration of various modeling applications: Excel, MatLab, and MathCad
  - Interchangeability of system components ("Plug-n-Play")
  - ISRU systems are easily updated

- **Functionality:**
  - Evaluation and of different O2 production processes and Excavation systems: mass, power, volume
  - Identify key parameters
  - Evaluate system performance
  - Identify design needs and improvements

- **Utility:**
  - Prove feasibility of ISRU
  - Support mission architecture studies
  - Support hardware development
Description of oxygen production processes: Carbothermal Reduction – PEM Electrolyzer

- **Hopper**
- **Excavator**
- **Auger**
- **Solar Concentrator**
- **Process gas storage tank**
- **Pump**
- **Condenser**
- **Water Pump**
- **H₂/H₂O separator & storage tank**
- **PEM Electrolyzer**

**Diagram Details:**
- Non-vacuum
- Vacuum
- H₂O
- CH₄
- CH₄ buffer tank
- ZnO → ZnS
- SO₂
- Regolith
- Vacuum
- Condenser
- Dryer
Description of oxygen production processes: H₂ Reduction – PEM Electrolyzer

Q: indicates heat added or removed
* Indicates optional component

Notes:
1. Can be multiple reactor assemblies

Valve (2-way)
Valve (3-way)
Regulator
Description of oxygen production processes:
H₂ Reduction – SO Electrolyzer

- H₂/H₂O storage tank* (see note 4)
- Compressor
- H₂/H₂O Separator (gas phase)
- Mixer
- SOE Electrolyzer
- Oxygen storage
- Q

Notes:
1. Can be multiple reactor assemblies
2. SOE can be operated slightly exothermic in which case outlet H₂O and H₂ can gain temperature.
3. Separating H₂ and H₂O before electrolyzer may make electrolyzer more efficient, but requires extra separator.
4. See chart 5 for a possible 2-reactor configuration/operation that may eliminate need for separate H₂/H₂O storage tank between batches.
Description of oxygen production processes: Electrolyzer Sub-system

- **Solid-Oxide**
  - Water electrolyzer → O₂
  - Species separator
  - H₂O, H₂

- **Cathode-fed PEM**
  - Heat exchanger
  - Water electrolyzer → O₂
  - Species separator
  - H₂

- **Anode-fed PEM**
  - Heat exchanger
  - Water electrolyzer
  - H₂
  - O₂, H₂O
  - Dryer
  - H₂O
  - O₂
System Model: A Modular Approach
ISRU System Level

Mission Requirements:
- Number of missions
- Number of EVAs
- Description of outpost

ISRU System Output:
- System Mass
- System Volume
- System Power

Inputs:
- Oxygen production rate
- Location of O₂ plant
- O₂ production process

O₂ Production System

Inputs:
- Regolith excavation rate
- Location of excavation site
- Location of O₂ plant
- Type of excavator/transporter

Excavation System

Outputs:
- Regolith required
- System mass
- System power
- System volume
System Model: A Modular Approach
O₂ Production and Excavation System Level

- Oxygen production system is divided into modules or unit operations
- Excavation system is divided into a force module and mass module
- Each module is modeled in a standalone Excel workbook using Visual Basics for Application (VBA)
- An Excel worksheet functions as the Input/Output interface (Databus)
- A VBA module is used to build a 'master' function where the calculations are performed
- Modules are linked using Phoenix Integration ModelCenter
- Each link represents information passed from one module to the other
  - The information is passed in the form of
    - individual cell
    - array of cells
  - Each cell or groups of cells is given a specific name (aka: Named Range)

<table>
<thead>
<tr>
<th>Module</th>
<th>Molten Regolith Electrolysis</th>
<th>H₂ Reduction</th>
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<th>Components</th>
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<td>Hopper</td>
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<td>Regolith Handling</td>
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<td>X</td>
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<td>Auger, auger-heat exchanger</td>
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<td>Electrolysis cell</td>
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<td>Reactor chamber, electrode, cathode</td>
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<td>Carbothermal reduction reactor</td>
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<td></td>
<td></td>
<td>Reactor chamber, rake system</td>
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<td>Methanation reactor</td>
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<td>X</td>
<td>Packed bed reactor</td>
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<tr>
<td>H₂ reduction reactor</td>
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<td>X</td>
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<td>Reactor chamber (fluidized or rotating bed)</td>
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<td>Gas feed system</td>
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<td>X</td>
<td>Supply storage tank, system gas storage tank, compressor</td>
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<td>Electrolyte recovery system</td>
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<td>Micro-channel heat exchanger</td>
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<td>Water condenser</td>
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<td>Water condenser</td>
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<td>Solar concentrator</td>
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</table>
System Model: A Modular Approach

O₂ Production System Level cont'd

There is a hierarchy in the Databus:

- **Inputs:**
  - **GlobalInput:** all constants and quantities that are specified at the system level
    - Location
    - Required O₂ Production
  - **DesignInput:** all other input parameters required to run a component but are not generated by other model components
    - Vessel diameter
    - Material of construction
  - **Inflow:** input values that describe fluid stream condition and composition
    - Temperature
    - Pressure
    - Flow rates (H₂, H₂O, O₂, CH₄, CO₂, CO, H₂S, Ar)
  - **Interface:** all other input values a component requires that come from another component
    - Reaction Time
    - Batch Time
    - Initial Soil Temperature

- **Outputs:**
  - **GlobalOutput:** all calculated values pertinent to overall model's conclusions
    - Mass
    - Power
    - Volume
  - **Outflow:** output values that describe fluid stream condition and composition
    - Temperature
    - Pressure
    - Flow rates (H₂, H₂O, O₂, CH₄, CO₂, CO, H₂S, Ar)
  - **DesignOutput:** all other calculated output values that describe component specifics but are not required by other components
    - Vessel height
    - Element mass

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### Table

<table>
<thead>
<tr>
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<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
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<td>6</td>
<td>Shuckleton Film (short nights)</td>
<td>Location of Power System</td>
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<td>Flag to specify primary input driver</td>
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<td>Desired O₂ production per year</td>
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<td>Average density of solid</td>
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<td>15</td>
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<td>%</td>
<td>FeO percent of solid by mass</td>
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<tr>
<td>16</td>
<td>2.000000</td>
<td>%</td>
<td>Sulfur percent of solid by mass</td>
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<td>17</td>
<td>0.000000</td>
<td>hr</td>
<td>Time to heat up 1 batch of regolith</td>
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<tr>
<td>18</td>
<td>12.000000</td>
<td>batches/day</td>
<td>Number of batches run per 24 hour day</td>
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<td>Material of Construction for Reactor and Cyclone</td>
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<td>Diameter (inside) of reactor</td>
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<td>21</td>
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<td>Insulation thickness</td>
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<td>24</td>
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<td>Void fraction in fixed bed</td>
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<td>26</td>
<td>0.400000</td>
<td>Void fraction in incipiently fluidized bed</td>
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<tr>
<td>27</td>
<td>0.500000</td>
<td>Void fraction in fluidized or loosely packed bed</td>
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<td>28</td>
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<td>m/s</td>
<td>Cyclone inlet velocity (95 m/s recommended)</td>
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<td>29</td>
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<td>Initial solid temperature</td>
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<td>Inlet temperature of gases</td>
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<td>31</td>
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<td>h₂ molar flow rate in</td>
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<td>CO molar flow rate in</td>
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<td>CO₂ molar flow rate in</td>
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<td>N₂ molar flow rate in</td>
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<td>mol/s</td>
<td>Inert molar flow rate in</td>
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</tbody>
</table>

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### Table

| B     | C    | Units | Description                              | named Range    |                 |
|-------|------|-------|-------------------------------------------|-----------------|
| 41    | Value| Vessel | Height                                     |                 |
| 42    | 1.92000 | m | Vessel Height                              |                 |
| 43    | 0.16000 | m | Vessel Diameter                           |                 |
| 44    | 0.00000 | m | Heaters plug diameter                      |                 |
| 45    | 1.28000 | kg | mass of reactor structure                 |                 |
| 46    | 0.02449 | kg | volume of reactor structure               |                 |
| 47    | 2.57909 | kg | mass of insulation                         |                 |
| 48    | 0.00471 | kg | volume of insulation                       |                 |
| 49    | 0.02350 | kg | mass of the cyclone structure             |                 |
| 50    | 0.00001 | kg | volume of the cyclone structure           |                 |
| 51    | 0.00000 | mol/s | required flow rate of hydrogen into reactor |                 |
| 52    | 0.00000 | mol/s | required regolith in reactor per batch     |                 |
| 53    | 0.00000 | mol/s | required time to react each batch of solids |                 |
| 54    | 0.00000 | mol/s | required time to heat solids to reaction temperature | |
| 55    | 0.87900 | K | Insulation heat lost                       |                 |
| 56    | 0.02000 | K | Endothermic heat loss                      |                 |
| 57    | 0.00000 | mol/s | energy required per batch to heat up solids |                 |
| 58    | 190.00000 | K | Outlet temperature                        |                 |
| 59    | 176317.000 | Pa | Outlet pressure                           |                 |
| 60    | 0.04427 | mol/s | h₂ molar flow rate out                    |                 |
| 61    | 0.00000 | mol/s | h₂O molar flow rate out                   |                 |
| 62    | 0.00000 | mol/s | CO molar flow rate out                    |                 |
| 63    | 0.00000 | mol/s | CO₂ molar flow rate out                   |                 |
| 64    | 0.00000 | mol/s | CO₂ molar flow rate out                   |                 |
| 65    | 0.00000 | mol/s | O₂ molar flow rate out                    |                 |
| 66    | 0.00000 | mol/s | h₂O molar flow rate out                   |                 |

---

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| 62    | 0.00000 | mol/s | CO molar flow rate out                    |                 |
| 63    | 0.00000 | mol/s | CO₂ molar flow rate out                   |                 |
| 64    | 0.00000 | mol/s | CO₂ molar flow rate out                   |                 |
| 65    | 0.00000 | mol/s | O₂ molar flow rate out                    |                 |
| 66    | 0.00000 | mol/s | h₂O molar flow rate out                   |                 |
System Model: A Modular Approach
O₂ Production Sub-System Level

- The Named Range creates a common interface for the modules
- This common interface enables the modules to be plug-n-play
ISRU System Model Tool: Sub-systems Description

- **Excavation sub-system:**
  - Force module calculates forces on digging tools and wheels/tracks based on classical soil mechanics correlations; dimensions of digging tool, wheels, and chassis; and power/energy requirements for digging and driving operations.
  - Mass module calculates the mass of individual components (digging tool, boom arm, motors & actuators, chassis, etc.) based on the dimensions and forces calculated in force module.
  - Options for bucket wheel, front-end loader, backhoe, and bull-dozer blade.
  - Options for wheels or tracks.
  - Options for continuous or intermittent digging. Capability to vary vehicle velocity, depth of cut, soil properties, surface slope (for driving), digging rate (e.g., regolith per day), per-delivery load, down-time between deliveries, and many other variables.

- **Regolith Handling sub-system:**
  - Includes feed and dump hoppers and augers.
  - Hoppers are sized based on amount of regolith stored.
  - Augers have an option for heat exchange between the feed auger (cold regolith) and dump auger (hot-spent regolith).

- **Reactor sub-system:**
  - Options for carbothermal processing, hydrogen reduction processing, and molten regolith electrolysis.
  - Carbothermal processing option includes a carbothermal reactor, desulfurization unit, and methanation reactor.
  - Carbothermal reactor, desulfurization, and methanation reactor models are based on recent design concepts.
  - Hydrogen reduction processing option includes a hydrogen reduction reactor and desulfurization unit. Hydrogen reduction reactor has options for a fluidized bed, loosely-packed bed, and a rotating bed (currently being developed).

- **Electrolyzer sub-system:**
  - Options for proton exchange membrane (PEM) and solid oxide (SO) electrolyzer.
  - PEM electrolyzer option includes a micro-channel heat exchanger, condenser, water pump, phase separator, PEM electrolyzer, and a water absorption bed.
  - SO electrolyzer option includes gas phase separators and SO electrolyzer.

- **Liquefaction sub-system:**
  - The liquefaction sub-system includes radiators, cryocoolers, and storage tanks. This sub-system has an option for single or multiple cryocoolers for condensing the oxygen produced and managing boil-off.

- **Thermal Energy sub-system:**
  - The thermal energy sub-system includes a rigid solar concentrator to provide thermal energy to the reactors. An inflatable solar concentrator option is currently being developed.
ISRУ System Model Tool: Summary of Inputs

- System model optimization:
  - Objective Definition:
    - minimize system mass
  - Design Variables:
    - Mass of regolith per batch
    - Time to heat up one batch
    - Reactor diameter
    - Number of batches per day
- Location:
  - Equatorial & Polar region
- Excavation sub-system:
  - Single scoop front-end loader, 6 wheels, and combined dig/haul vehicle(s)
  - Intermittent digging (i.e., downtime between deliveries) selected to minimize total energy
- Regolith Handling sub-system:
  - No heat exchanger
- Reactor sub-system:
  - Carbothermal processing
  - Hydrogen reduction processing: 2-fluidized bed for continuous operation
- Electrolyzer sub-system:
  - Proton exchange membrane (PEM)
- Liquefaction sub-system:
  - 1-cryocooler
  - 2-storage tanks
- Thermal Energy sub-system:
  - Rigid solar concentrator
ISRU System Model Tool: 
System Mass Results

- All ISRU system mass show a linear dependency with respect to oxygen production.
- Carbothermal @ Polar < @ Equatorial:
  - No dependency on regolith composition
  - Operating: Polar = 255 days/yr vs Equatorial = 183 days/yr
- H2 reduction @ Polar > @ Equatorial:
  - Dependency on regolith composition: FeO = 15% equatorial vs 5% polar
  - Even though operating time in equatorial region is less, the effect of regolith composition on the overall system mass is greater than the operating time.
- Mass payback is achieved after the first six months of deployment on either O2 production system.
### ISRU System Model Tool: Mass Breakdown - Polar Region

<table>
<thead>
<tr>
<th></th>
<th>H2 Reduction - Polar Region</th>
<th>Carbothermal Reduction - Polar Region</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1MT/yr</td>
<td>5MT/yr</td>
</tr>
<tr>
<td></td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Percent of total mass</td>
<td>84</td>
<td>236</td>
</tr>
<tr>
<td></td>
<td>90%</td>
<td>64</td>
</tr>
<tr>
<td></td>
<td>80%</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>70%</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>60%</td>
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<td></td>
<td>50%</td>
<td>155</td>
</tr>
<tr>
<td></td>
<td>40%</td>
<td>214</td>
</tr>
<tr>
<td></td>
<td>30%</td>
<td>466</td>
</tr>
<tr>
<td></td>
<td>20%</td>
<td>675</td>
</tr>
<tr>
<td></td>
<td>10%</td>
<td>601</td>
</tr>
<tr>
<td></td>
<td>0%</td>
<td>0</td>
</tr>
</tbody>
</table>

Numbers on the columns represent the mass of the sub-system in kilograms

- Inefficiency of H2 reduction is seen on the mass of excavation sub-system and regolith handling sub-system
- Mass of thermal energy, electrolysis, and liquefaction sub-systems in H2 reduction is reduced because multiple reactor sub-system is assumed allowing continuous processing (no downtime)
- As oxygen production rate increases the fidelity of the reactor sub-system model decrease
  - More noticeable in carbothermal model
  - Available experimental data is targeted to low production rate
Downtime at Equatorial region is greater than at Polar region
- The effect of operating time is greater in carbothermal than in H2 reduction due to multiple reactors on H2 reduction system
Summary & Conclusions

- ISRU System Model Tool:
  - has been develop for the analysis of ISRU systems: Excavation and O2 production
  - is flexible, and allows any component model developed in various applications to be integrated into the model environment as long as the model meets interface requirements

- The ISRU System Model Tool has been successfully used to provide ISRU system mass, power, and volume estimates to architecture studies

- Models are validated with available experimental data at low production rates; experimental data at higher production rates is needed.

- ISRU System Model Tool mass estimates results show that mass payback is achieved within six months of operation
  - Including H2 reduction with Mare-type regolith (~5% FeO)
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ISRU System Model Tool Demo
Questions?