ISRU SYSTEM MODEL TOOL: FROM EXCAVATION TO OXYGEN PRODUCTION. E. Santiago-Maldonado[1] and D. L. Linne[2], [1]NASA KSC Mail Code KT-D Kennedy Space Center, FL 32828, Edgardo.Santiago-Maldonado-1@nasa.gov, [2]NASA 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 ISMT is capable of performing optimization on an ISRU system composed of one option of each subsystem. Furthermore, the ISMT allows for trade studies of each system configuration by replacing any option within each sub-system.

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

Acknowledgment:
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References:

[1] Conceptual Design of a Lunar Oxygen Pilot Plant Lunar Base Systems Study (LBSS) Task 4.2 (Eagle Engineering Inc) (NASA-CR-172082)
[2] Phoenix Integration Inc, "ModelCenter: Desktop Trade Studies." http://www.phoenix-int.com/products/modelcenter.php ; 9/13/2007
[3] Gustafson, R., "Phase I final report: Carbothermal Reduction of Lunar Regolith." NASA contract NNJ05HB57C, 2006
[4] Clark, L. "Integrated In-Situ Resource Utilization for Human Exploration – Propellant for the Moon and Beyond: Phase 1 Final Report." NASA contract NNJ05HB57C, 2006

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ISRU System Model Tool: From Excavation to Oxygen Production

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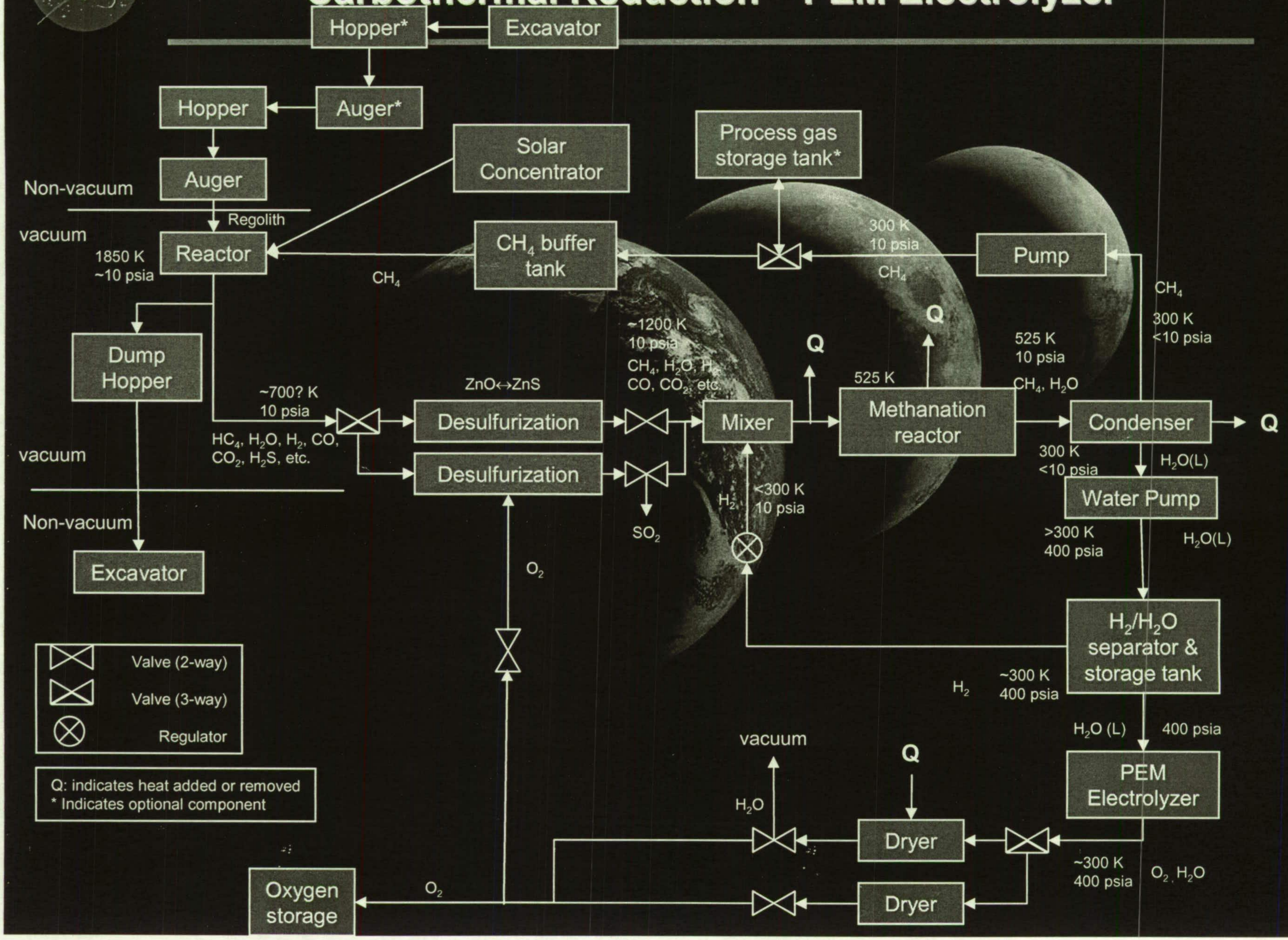
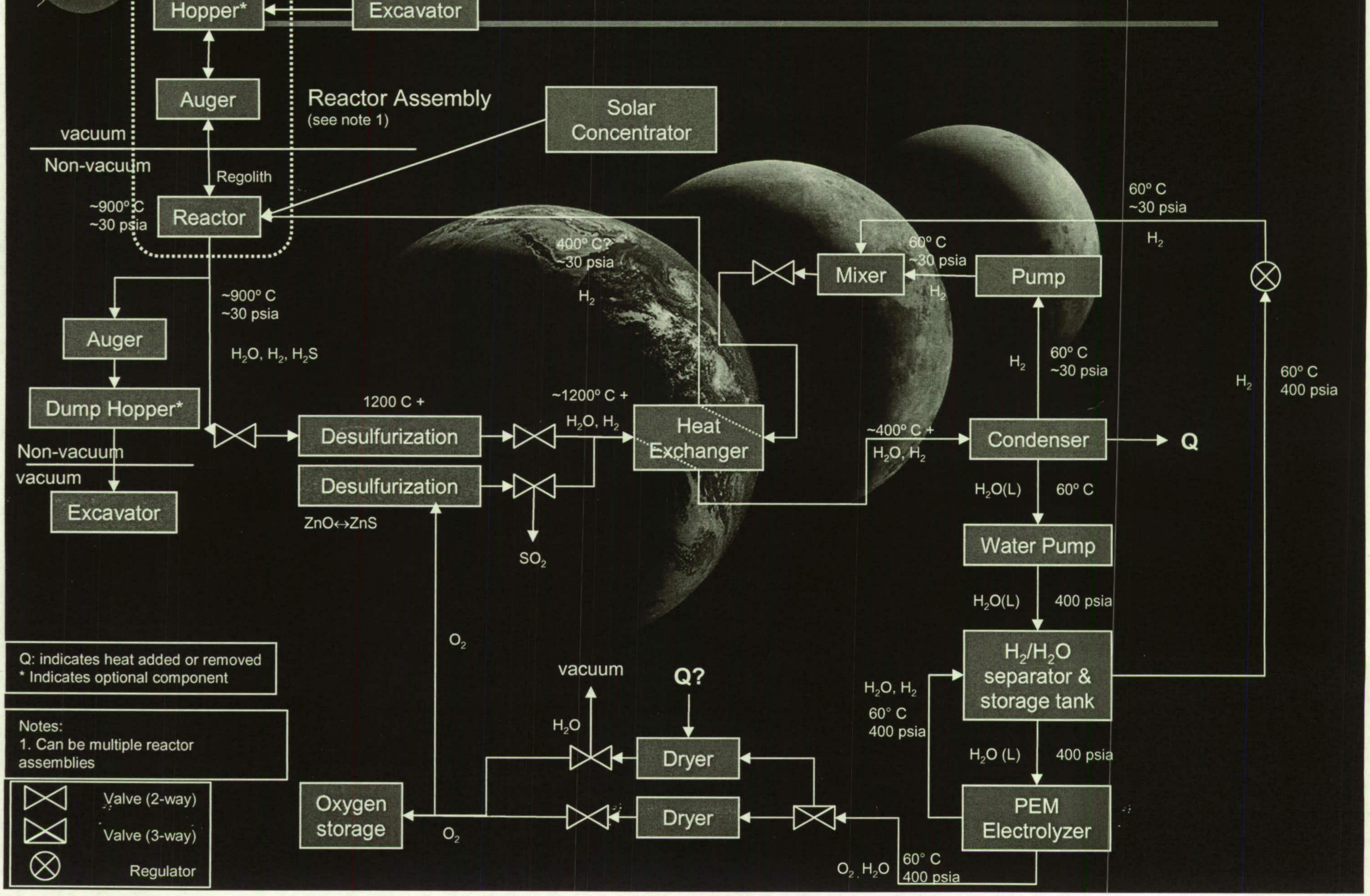
ISRU System Model Tool

- 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

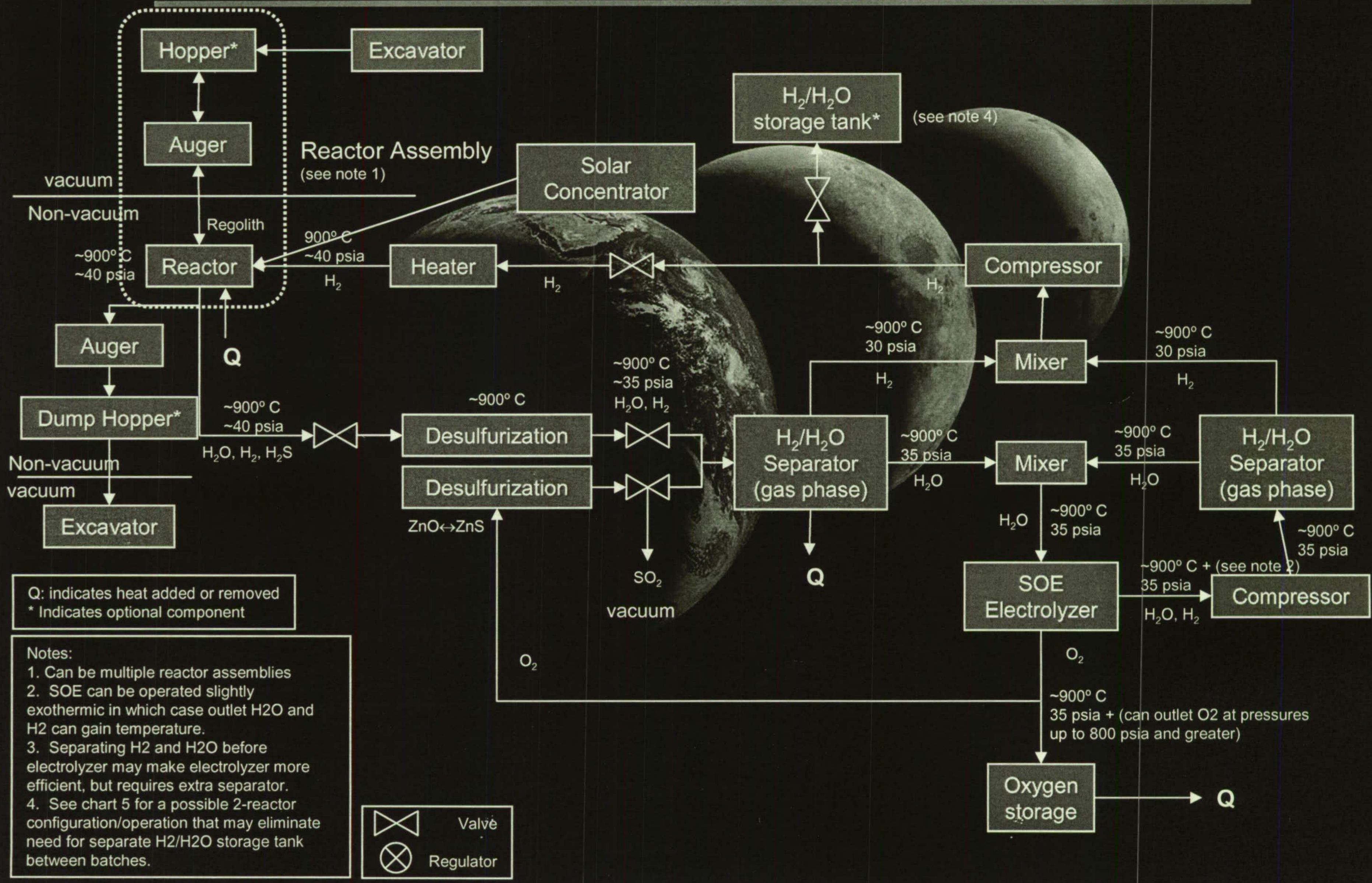
Description of oxygen production processes: Carbothermal Reduction – PEM Electrolyzer



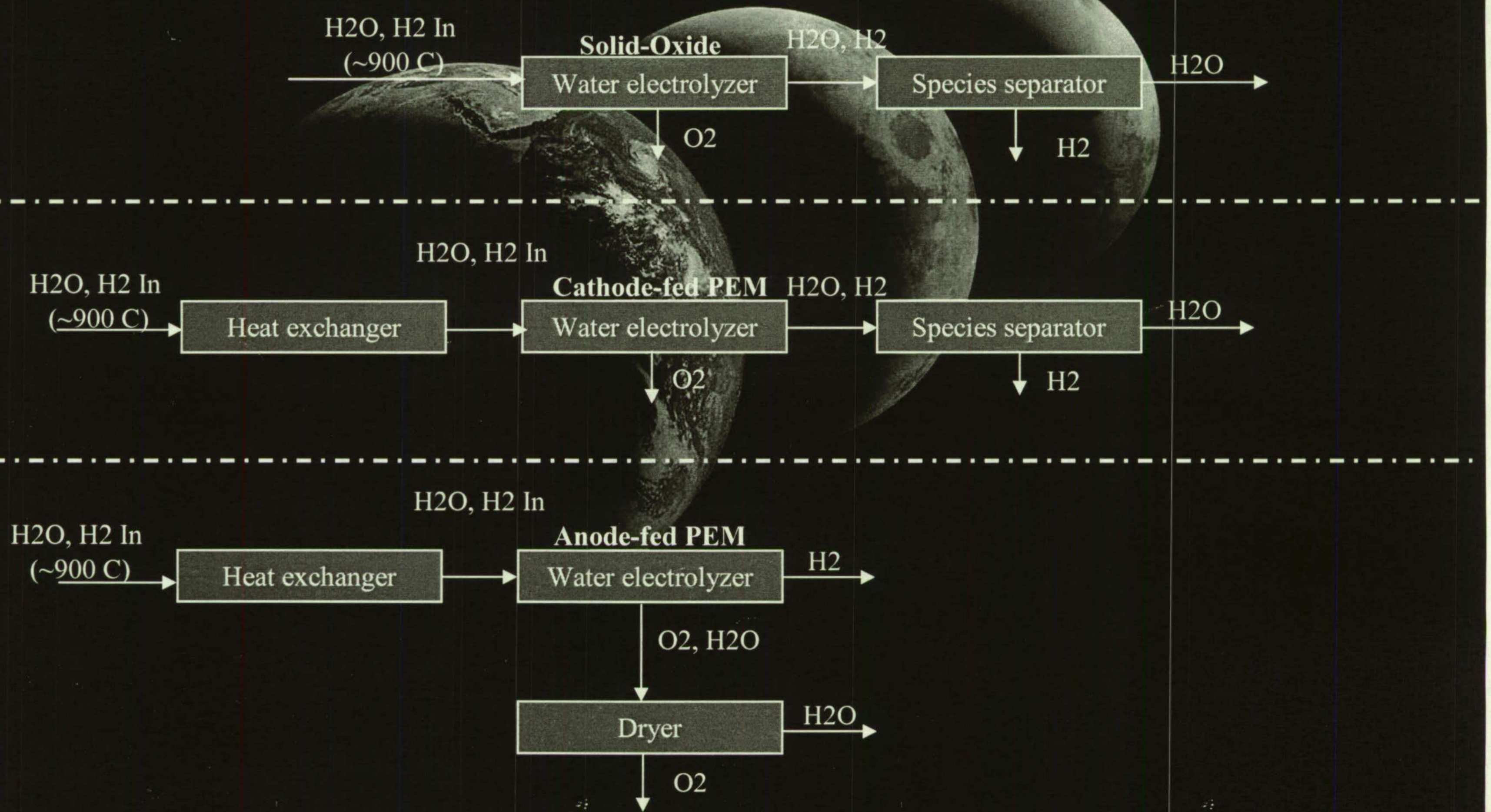
Description of oxygen production processes: H_2 Reduction – PEM Electrolyzer



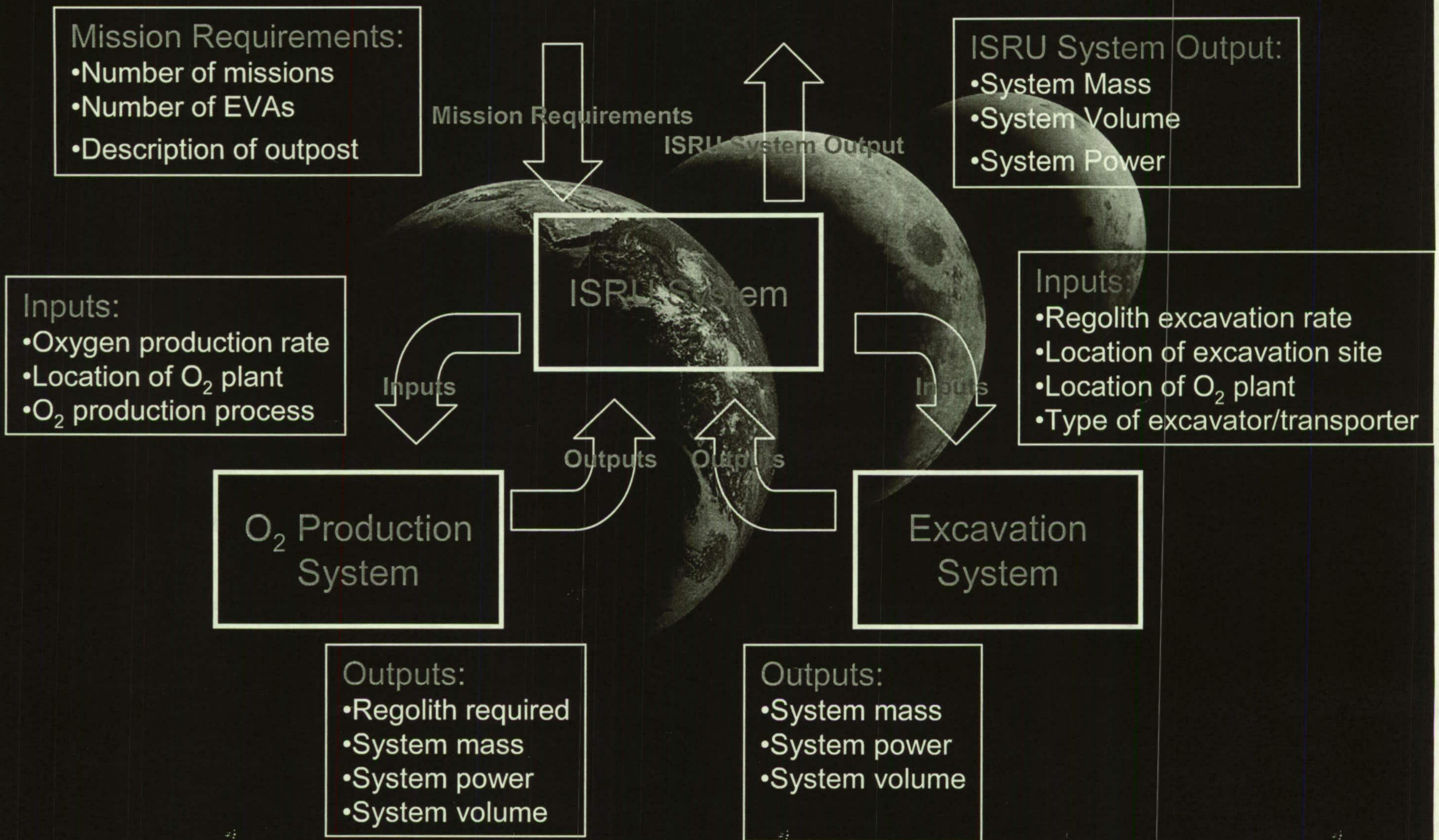
Description of oxygen production processes: H_2 Reduction – SO Electrolyzer



Description of oxygen production processes: Electrolyzer Sub-system



System Model: A Modular Approach
ISRU System Level



System Model: A Modular Approach
O_2 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 stand-alone 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)

Module	Molten Regolith Electrolysis	H2 Reduction	Carbothermal	Components
Hopper	X	X	X	Hopper
Regolith Handling	X	X	X	Auger, auger-heat exchanger
Electrolysis cell	X			Reactor chamber, electrode, cathode
Carbothermal reduction reactor			X	Reactor chamber, rake system
Methanation reactor			X	Packed bed reactor
H2 reduction reactor		X		Reactor chamber (fluidized or rotating bed)
Gas feed system		X	X	Supply storage tank, system gas storage tank, compressor
Electrolyte feed system	X			Supply storage tank,
Electrolyte recovery system	X			Supply storage tank,
Heat exchanger		X	X	Micro-channel heat exchanger
Water condenser		X	X	Water condenser
Water Electrolyzer		X	X	PEM and solid oxide electrolyzer, water pumps
Water removal unit		X	X	Water removal unit
De-sulfurization unit	X	X	X	De-sulfurization unit
Solar concentrator		X	X	Solar concentrator, fiber optics

System Model: A Modular Approach
O_2 Production System Level cont'd

There is a hierarchy in the Databus:

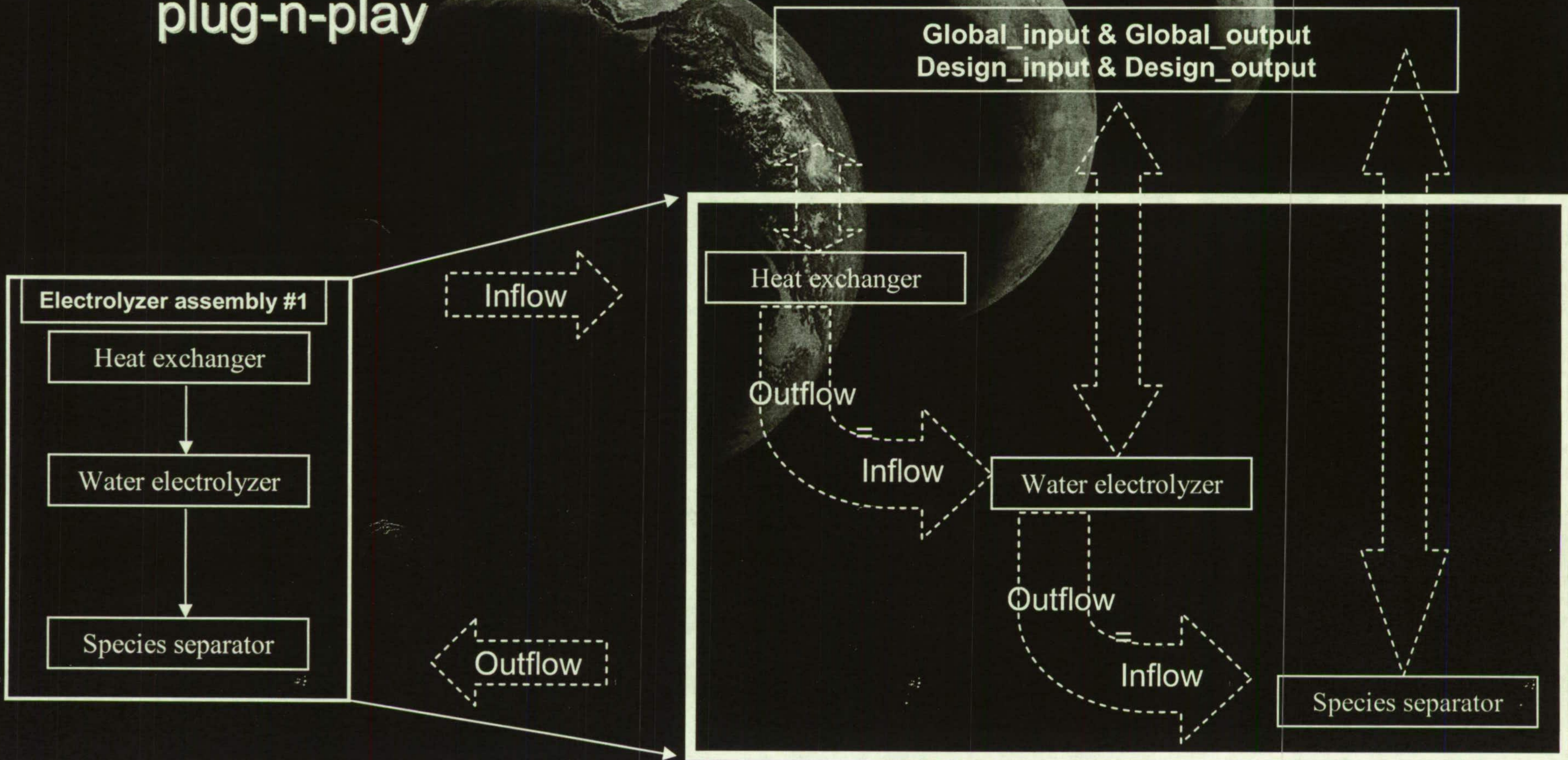
- **Inputs:**
  - **GlobalInput:** all constants and quantities that are specified at the system level
    - Location
    - Required O2 Production
  - **DesignInput:** all other input parameters required to run a component but are not generated by other model components
    - Vessel diameter
    - Material of construction
  - **Inflow:** input values that describe fluid stream condition and composition
    - Temperature
    - Pressure
    - Flow rates (H_2, H_2O, O_2, CH_4, CO_2, CO, H_2S, 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: out**put values that describe fluid stream condition and composition
    - Temperature
    - Pressure
    - Flow rates (H_2, H_2O, O_2, CH_4, CO_2, CO, H_2S, Ar)
  - **DesignOutput:** all other calculated output values that describe component specifics but are not required by other components
    - Vessel height
    - Element mass

	B	C	D	E	F
3	Input Field				
4	Value	Units	Description	named Range	
5	Shackleton Rim (short nights)		Location of Power System		
6	Solar (day only)		Power Type		
7	1.63000	m/s2	Gravity Constant		
8	Input Solids per Batch		Flag to specify primary input driver		
9	15.00000	kg	Solid mass in reactor per batch		
10	1000.00000	kg	Desired O2 production per year		
11	0.80000		Regolith particle sphericity		GlobalInputs
12	0.00000	m	Smallest particle size		
13	0.00020	m	Largest particle size		
14	3000.00000	kg/m3	Average density of solid		
15	5.00000	%	FeO percent of solid by mass		
16	0.20000	%	Sulfur percent of solid by mass		
17	0.50000	hr	Time to heat up 1 batch of regolith		
18	12.00000	batches/day	Number of batches run per 24 hour day		
19	Al 2014-T6		Material of Construction for Reactor and Cyclone		
20	2.00000		Safety factor for Reactor shell		
21	2.00000		Safety factor for cyclone		
22	0.16400	m	Diameter (inside) of reactor	ModuleInput	
23	0.02000	m	Insulation thickness		
24	Fluidized		Type of reactor bed		DesignInputs
25	0.30000		Void fraction in fixed bed		
26	0.40000		Void fraction in inciepently fluidized bed		
27	0.50000		Void fraction in fluidized or loosely packed bed		
28	15.00000	m/s	Cyclone inlet velocity(15 m/s recommended)		
29	425.00000	K	Initial solid temperature		InterfaceIn
30	1100.00000	K	Inlet temperature of gases		
31	206843.00000	Pa	Inlet pressure of gases		
32	0.04800	mol/s	h2 molar flowrate in		
33	0.00000	mol/s	h2o molar flowrate in		
34	0.00000	mol/s	o2 molar flowrate in		
35	0.00000	mol/s	ch4 molar flowrate in		ModuleInflow
36	0.00000	mol/s	co2 molar flowrate in		
37	0.00000	mol/s	co molar flowrate in		
38	0.00000	mol/s	h2s molar flowrate in		
39	0.00000	mol/s	inert molar flowrate in		
40	Output Field				
41	Value	Units	Description	named Range	
42	1.15929	m	Vessel Height		
43	0.16400	m	Vessel Diameter		
44	0.09086	m	Heater Rod diameter		
45	1.62182	kg	mass of reactor structure		
46	0.02449	m3	volume of reactor structure		
47	3.57008	kg	mass of insulation		
48	0.01471	m3	volume of insulation		
49	0.02350	kg	mass of the cyclone structure		
50	0.00044	m3	volume of the cyclone structure		DesignOutput
51	0.04670	mol/s	required flow rate of hydrogen into reactor		
52	15.00000	kg	required regolith in reactor per batch		
53	1.18013	hr	required time to react each batch of solids		
54	0.50000	hr	required time to heat solids to reaction temperature		
55	0.87856	KW	insulation heat loss		
56	0.02865	KJ	endothermic heat loss	ModuleOutput	
57	11562.22982	KW	energy required per batch to heat up solids		
58	1100.00000	K	outlet temperature		
59	176317.56203	Pa	outlet pressure		
60	0.04427	mol/s	h2 molar flowrate out		
61	0.00221	mol/s	h2o molar flowrate out		
62	0.00000	mol/s	o2 molar flowrate out		ModuleOutflow
63	0.00000	mol/s	ch4 molar flowrate out		
64	0.00000	mol/s	co2 molar flowrate out		
65	0.00000	mol/s	co molar flowrate out		
66	0.00022	mol/s	h2s molar flowrate out		

System Model: A Modular Approach
O_2 Production Sub-System Level

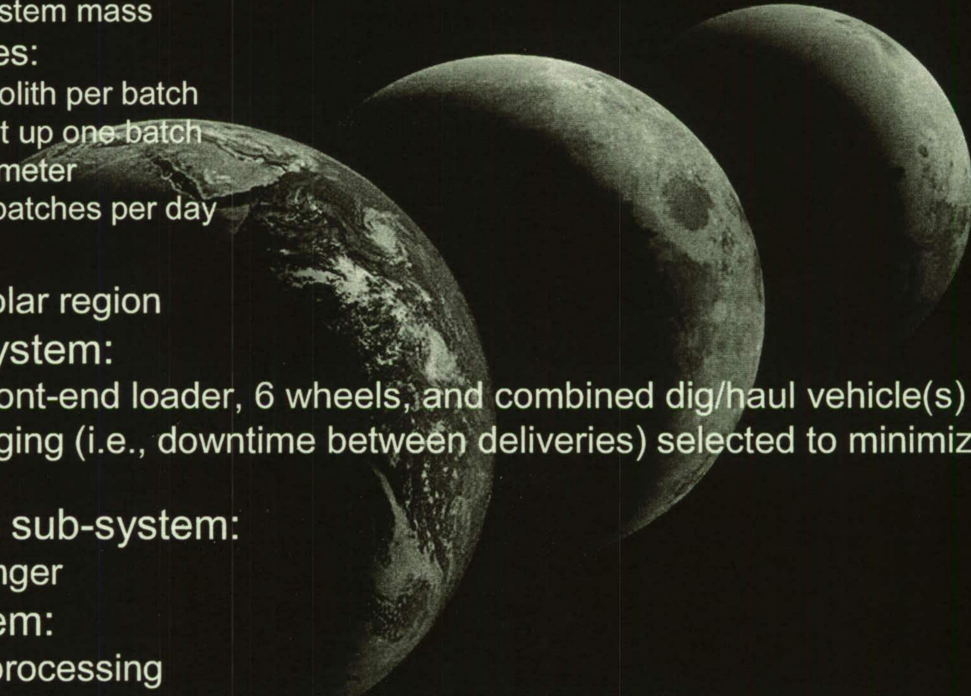
- The Named Range creates a common interface for the modules
- This common interface enables the modules to be plug-n-play



ISRU System Model Tool: Sub-systems Description

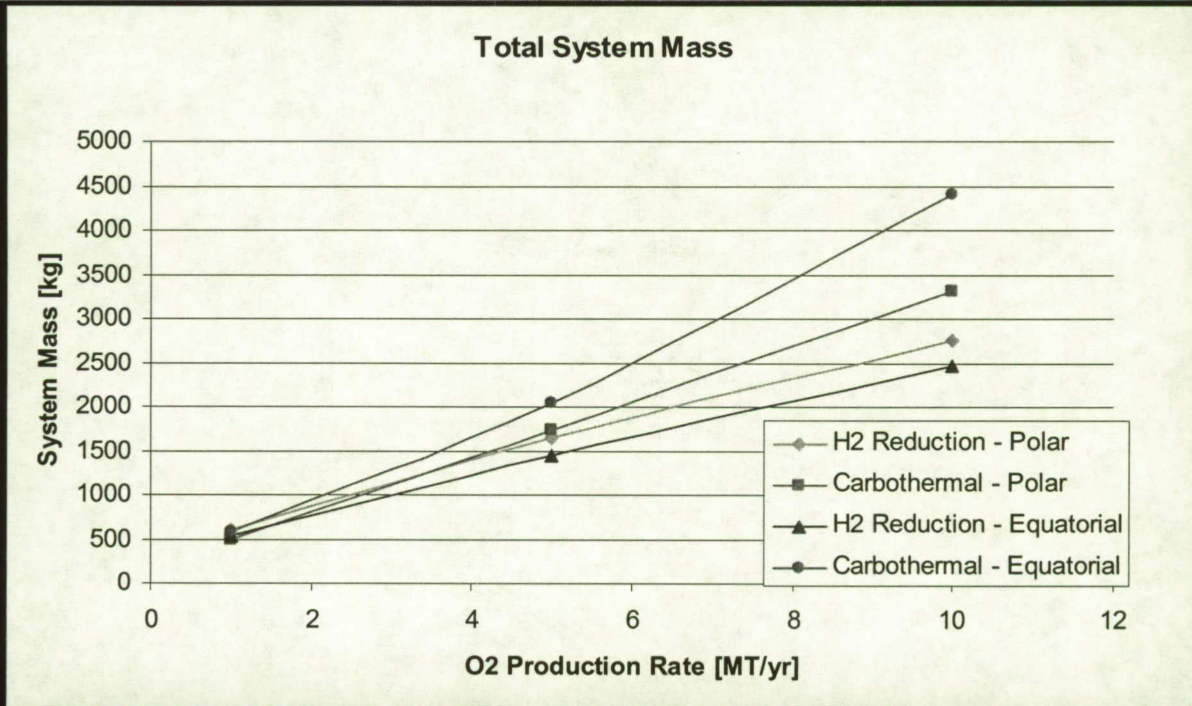
- Excavation sub-system:
  - Force module calculates forces on digging tools and wheels/tracks based on classical soil mechanics correlations; dimensions of digging tool, wheels, and chassis; and power/energy requirements for digging and driving operations.
  - Mass module calculates the mass of individual 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.

ISRU System Model Tool: Summary of Inputs



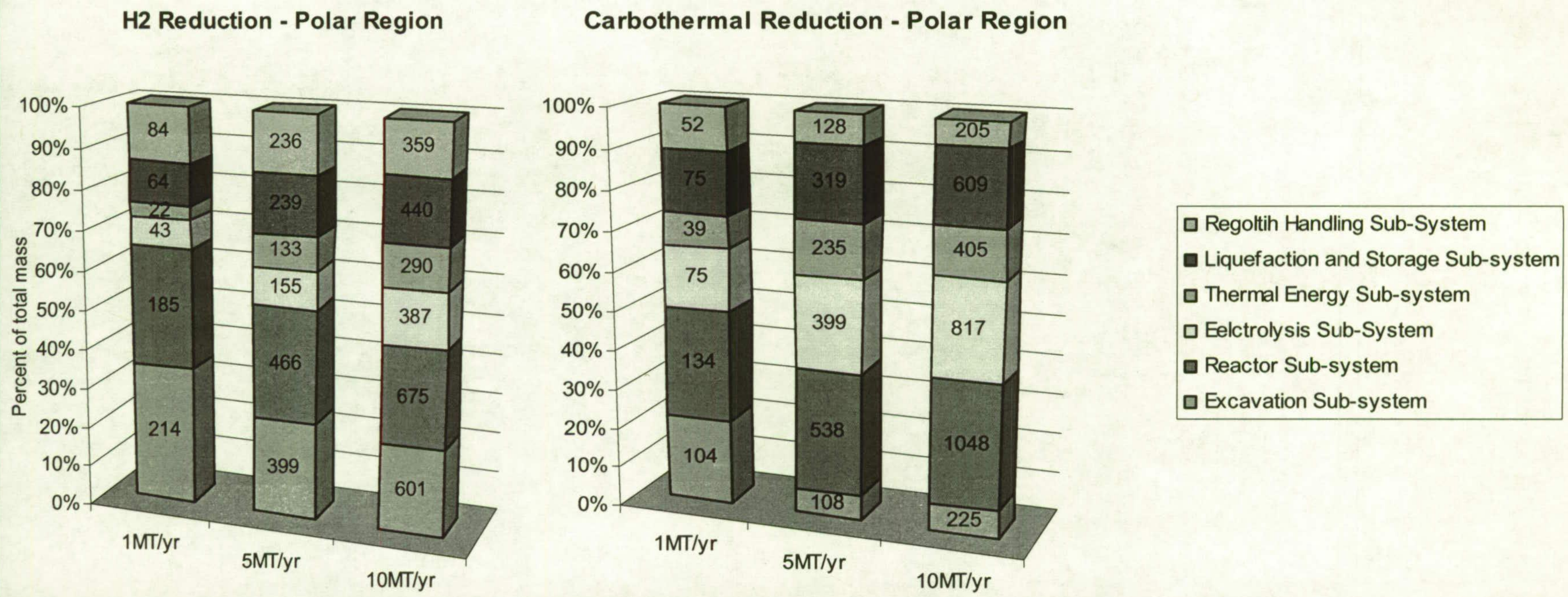
- System model optimization:
  - Objective Definition:
    - minimize system mass
  - Design Variables:
    - Mass of regolith per batch
    - Time to heat up one batch
    - Reactor diameter
    - Number of batches per day
- Location:
  - Equatorial & Polar region
- Excavation sub-system:
  - Single 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 liner 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

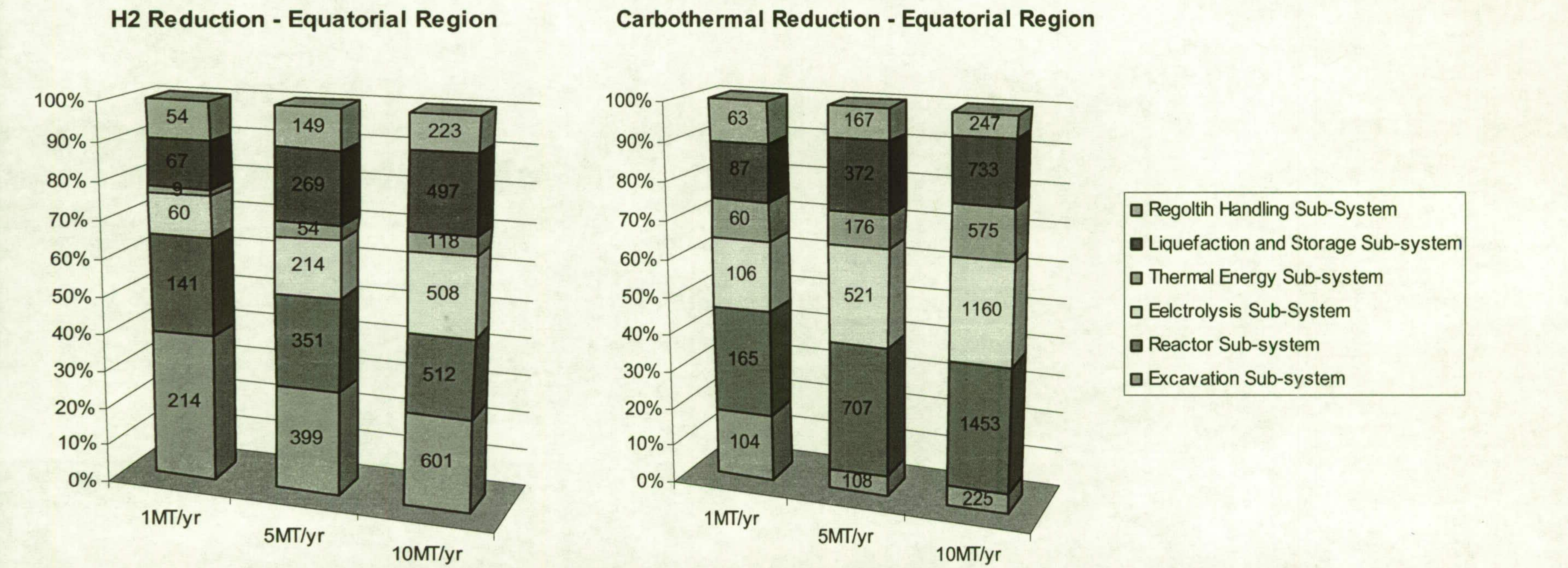
ISRU System Model Tool: Mass Breakdown - Polar Region



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

ISRU System Model Tool: Mass Breakdown – Equatorial Region



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

- 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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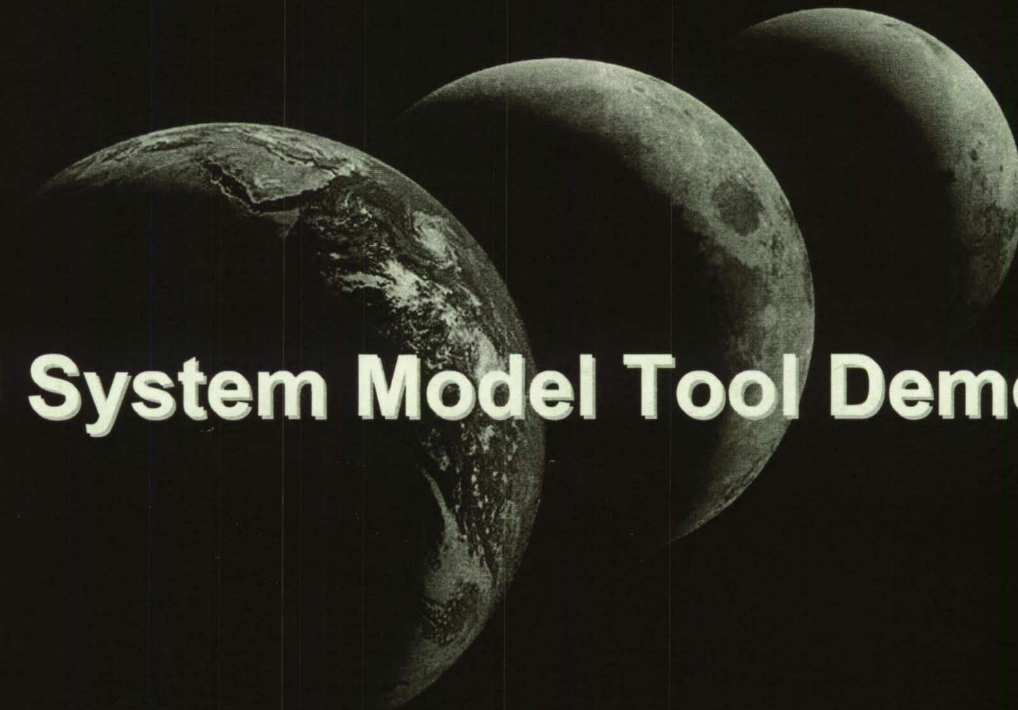
  - Robert Gustafson, Orbitec Technologies Corp.
  - Takashi Nakamura, Physical Sciences Inc.

ISRU System Model Tool Demo



Questions?