Integrated Bosch Process System Models for In-Situ Oxygen and Carbon Production

Beau M. Compton[1]
NASA Glenn Research Center, Cleveland, Ohio, 44135

Travis M. Wilson[2]
HX5, NASA Glenn Research Center, Cleveland, Ohio, 44135

Arland Zatania Lojo[3]
HX5, NASA Glenn Research Center, Cleveland, Ohio, 44135

Michael J. Cooper[4]
NASA Glenn Research Center, Cleveland, Ohio, 44135

In-Situ Resource Utilization (ISRU) technology is a vital component to NASA's mission of a sustainable presence on the Moon and Mars. Local resources can be leveraged to reduce resupply frequency and mass. Elements of the Bosch process, combined with the carbothermal reduction process, can produce oxygen on the lunar surface with minimal consumables. The Bosch process can also produce oxygen on the Martian surface by using the CO_2-rich environment. Between both systems, adsorption pump, solar thermal energy, carbon formation reactor, and water recovery subsystems are modeled and integrated to create a functional model in MATLAB software. The model is used to simulate performance of the system and reduce mass, power, and volume requirements. This integrated system model provides a tool to scale ISRU technologies for oxygen and carbon production.

The MATLAB model is created by developing a system of independent subsystem models that are solved for their quasi-steady state values which can be integrated with respect to time to determine the change in current states. A flexible time stepping method is used to ensure a high level of accuracy during periods of rapid change while still making use of a simple explicit integration method. The flexible time step is calculated for each independent subsystem and the minimum value from those is used as the overall time step. A flexible time step is calculated by dividing a resolution value, or the maximum change per time step, by the variables current rate of change. The maximum value from all points in space is used for subsystem models that contain multiple values. The process is done for every variable that is being monitored in each subsystem and the global minimum is used as that iteration's timestep. Several assumptions used in the MATLAB model for fluid flow dynamics, such as 1-D gas flow through the sorption pump, are supported by modeling in Ansys Fluent software.

[1] Aerospace Engineer, Chemical and Thermal Propulsion Systems
[2] Aerospace Engineer, Chemical and Thermal Propulsion Systems
[3] Aerospace Engineer, Chemical and Thermal Propulsion Systems
[4] Aerospace Engineer, Chemical and Thermal Propulsion Systems

The Lunar oxygen production system is outlined in Fig. 1. The carbothermal reduction subsystem uses solar energy to heat a mixture of lunar regolith and carbon powder to produce carbon monoxide. To begin, the carbon monoxide feeds to the modified Bosch subsystem along with hydrogen gas. The reactants then enter the carbon formation reactor where water and carbon powder are produced. Solar thermal energy is used to add energy to the reactor, but waste heat from the carbothermal process is another potential heat source. The water is collected and electrolyzed to produce hydrogen which reenters the Bosch subsystem, and the oxygen is stored for downstream use. The carbon powder is collected and feeds back into the carbothermal subsystem.

The Martian oxygen production system uses the full Bosch process and is outlined in Fig 2. A CO_2 adsorption pump thermally cycles to scrub and pressurize CO_2 from the environment. Along with an initial supply of hydrogen, the reactants enter the Reverse Water Gas Shift Reactor (RWGSR) which produces carbon monoxide and water. Carbon monoxide and unreacted hydrogen enter the carbon formation reactor to produce water and carbon powder. The water is collected from both reactors and electrolyzed to reintroduce hydrogen and store oxygen for propellant production or life support. Carbon is removed from the carbon formation reactor and stored.

The adsorption pump utilizes rapid cycle temperature swings within a stack of zeolite coated surfaces. The subsystem model solves 1-D quasi-steady conservation laws of the quasi-steady form, shown in Eq. 1, for the gas stream and heat exchange liquid to predict performance parameters such as breakthrough capacity and optimum cycle time. The source term S is used to capture interactions between the fluid flows and the sorbent. A quasi-steady-state scheme is used where no time derivatives appear in the governing equations, except for those in the source terms. This results in an autonomous system, where $\frac{\partial F}{\partial x} = \boldsymbol{f}(\boldsymbol{F})$. The fluxes F are provided at the inlet, and an explicit method is used to solve for the spatial distribution of F. The heat and mass flows to the sorbent are then extracted from the source terms. These flows are numerically integrated to produce a 1-D solution for the system's state as a function of both time and space. The body of the adsorption pump is separated into two semi-independent models: the heat exchanger fluid flow and gas flow through the zeolite coated surfaces. Both models are solved using the above-described method to find a 1-D solution as a function of space and interact only once a timestep is taken. The interaction point is the sorbent through which all heat transfer between the two models must occur. Sorbent mass adsorption is calculated using the Lagergren model, shown in Eq. 2, where the transfer coefficient, λ_D, is found by solving a system of nondimensionalized equations derived by using the heat and mass transfer analogy for transport phenomena. Using Grade 544 Type 13X zeolite as the sorbent material, the equilibrium concentration, θ_{eq}, is calculated using the k-site Langmuir isotherm and fit parameters. Additionally, the enthalpy of adsorption used in the model is computed by interpolation of available data [1]. The subsystem model was validated using the Rapid Cycle Temperature Swing Adsorption (RC-TSA) pump.

The solar thermal energy subsystem focuses on a solar concentrator concept with a heat exchanger to heat the reactants before entering the carbon formation reactor. The subsystem model assumes a fixed solar flux and reflector efficiency to calculate the reactant temperature given the incoming temperature, pressure, and exchanger geometry. The receiver is a custom manufactured series of copper blocks with serpentine channels to increase its surface area and the residence time of the reactants to heat up to 550 °C. The subsystem model was validated using a heat exchanger developed at NASA Glenn Research Center (GRC).

The carbon formation reactor facilitates several chemical reactions to produce water and carbon powder. It must operate at approximately 550 °C and the exothermic output must be understood to properly size the upstream heat exchanger. Additionally, an understanding of the catalysis and gas kinetics are important to understand the transport. The model was analytically and empirically derived from testing and validated using a carbon formation reactor developed by pH Matter, LLC.

I. Optional Supporting Materials

A. Images, Figures, and Tables

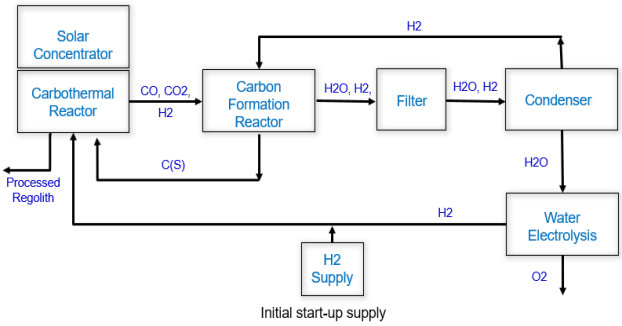

Fig. 1 Simplified Diagram of a Lunar Oxygen Production System

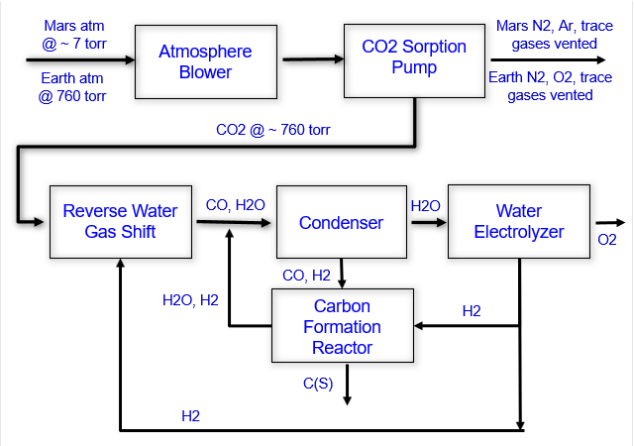

Fig. 2 Simplified Diagram of a Martian/Terrestrial Oxygen Production System

B. Equations

Eq. 1; $\frac{\partial F}{\partial x} = S(x,t)$

Eq. 2; $\frac{\dot{m}}{A} = \lambda_D(\theta_{eq} - \theta)$

C. References

[1] Cmarik, G.E., Son K.N., and Knox, J.C., "Standard Isotherm Fit Information for Dry CO2 on Sorbents for 4-Bed Molecular Sieve", NASA/TM—2017-219847