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Employing ISRU Models to Improve Hardware Design

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An analytical model for hydrogen reduction of regolith was used to investigate the effects of several key variables on the energy and mass performance of reactors for a lunar in-situ resource utilization oxygen production plant. Reactor geometry, reaction time, number of reactors, heat recuperation, heat loss, and operating pressure were all studied to guide hardware designers who are developing future prototype reactors. The effects of heat recuperation where the incoming regolith is pre-heated by the hot spent regolith before transfer was also investigated for the first time. In general, longer reaction times per batch provide a lower overall energy, but also result in larger and heavier reactors. Three reactors with long heat-up times results in similar energy requirements as a two-reactor system with all other parameters the same. Three reactors with heat recuperation results in energy reductions of 20 to 40 percent compared to a three-reactor system with no heat recuperation. Increasing operating pressure can provide similar energy reductions as heat recuperation for the same reaction times.

Nomenclature

d_p	=	particle diameter
f_s	=	particle sphericity
g	=	gravity constant
g	=	(subscript) gas
H/D	=	reactor height-to-diameter ratio
mf	=	minimum fluidization
s	=	solid
ε	=	void fraction
μ	=	viscosity
ρ	=	density

I. Introduction

NASA's current exploration vision includes plans to go back to the moon for extended stays to perform scientific research and exploration, and in preparation for future missions to Mars. To enable long duration stays of six months or more, it is imperative that technologies to reduce the required logistics and consumable resupply train from the Earth are developed. A leading candidate for reducing the consumables delivery from Earth is to learn to live off the land by utilizing in-situ resources. For example, oxygen can be extracted from the lunar regolith to provide breathing air for the habitat, airlock, and EVA suits, to provide propellant for the ascent vehicle or surface mobility vehicles such as hoppers, and eventually to ship to an in-space propellant depot in support of human missions to Mars. [1-3]

The concept of in-situ resource utilization (ISRU) has been proposed and studied since before the first moon landing,[4] and with the recent renewed effort toward returning to the moon the focus has turned toward the entire end-to-end oxygen production system.[5] This system focus, however, has only served to highlight how critical the reactor is to the entire operation. For the last few years, a multi-center NASA team has been developing analysis tools to increase the understanding of various components of an ISRU system, with a special emphasis on both the hydrogen reduction and carbothermal reduction reactors. This tool has already enabled the ISRU team to understand where peak power requirements develop, and how the use of parallel reactors, for example, can significantly reduce peak power by splitting up times for regolith heating and oxygen extraction.[6,7]

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The hydrogen reduction process has been the focus of the early end-to-end system efforts as it is the farthest along in development, although it produces the lowest yield of the many possible reduction concepts. However, it has been difficult for hardware designers to understand the complex interactions between the myriad parameters that they must select before building a prototype reactor. Previous analysis showed that processing larger regolith quantities in fewer batches per day significantly decreases the energy requirement and the total amount of regolith to be excavated and processed per day.[8] That analysis, however, kept several variables constant such as the number of reactors, the diameter of the reactor, the reactor operating temperature and pressure, and the initial temperature of the regolith. The design team for the next generation reactor has expressed a desire to better understand how these additional parameters should be determined from an overall performance perspective; therefore the analysis team has performed additional parametric analyses to help guide the hardware designers toward selection of a more optimal reactor system.

II. Hydrogen Reduction Reactor

The hydrogen reduction reaction involves heating the regolith to 800 – 1100 degrees C and reacting with gaseous hydrogen to extract oxygen from the iron-bearing minerals in the form of water. This water is then electrolyzed, with the oxygen being stored and the hydrogen being recycled back into the reactor. Current concepts for mixing the hydrogen and the regolith include a fluidized bed or a mechanical means to stir the regolith. The mixing causes the hydrogen gas to be well-dispersed and heat to be uniformly distributed. A model has been developed to analyze the physical, thermal, and chemical characteristics of these reactors during operation.[9]

Previous analysis evaluated a 2-reactor system, with one reactor extracting oxygen from the regolith while the second reactor was emptying spent regolith, filling with fresh regolith, and heating the regolith to operating temperature. This operating mode greatly reduces the total power requirement for the reactors by allowing much longer times to heat the regolith. This parallel reactor operation also provides more continuous gas flow rates to the electrolyzer and oxygen liquefaction systems downstream, thereby also reducing their mass and power. It has been postulated that heat-up power could be further reduced if a method was devised to transfer or recuperate some of the heat from the spent regolith to the incoming batch before dumping. One method the hardware designers would like to test is to recuperate this heat within the reactor hardware. This now introduces a third major operation to the reactor (heat-up, reaction, and recuperation), and suggests that three reactors might provide overall benefits.

To minimize power and energy required for the reactor system, both powered operations must be considered. The power during heat-up is dependent on the time allowed and the amount of regolith that needs to be brought up to temperature. Increasing the yield results in a reduction in total regolith that needs to be processed, and therefore a reduction in total heat-up energy. Power is also required to maintain temperature during reaction. Therefore, any parameters that affect the heat loss will affect power and energy required for reaction.

III. Fluidization

The hydrogen reduction model includes classical fluidization equations to calculate the amount of hydrogen flow required into the reactor to fully fluidize the regolith.[10] The minimum fluidization velocity is dependent on particle density and size, and gas density and viscosity as shown in Eq. (1):

$$u_{mf} = \frac{(\rho_s - \rho_g)}{150 * \mu_g} g d_p^2 \frac{(\varepsilon_{mf}^3 * f_s^2)}{1 - \varepsilon} \tag{1}$$

The actual flow velocity is generally chosen to be between the minimum fluidization velocity and the terminal velocity of a falling particle, which is also a function of viscosity and density. The flow rate of hydrogen required for fluidization is the flow velocity times the reactor cross sectional area and is therefore also strongly dependent on the reactor diameter. The total height of a fluidized bed reactor is dependent on the transport disengagement height, or the height at which most of the particles will fall out of the rising gas stream. For the conditions in the hydrogen reduction reactor, this typically is about twice the height of the quiescent bed, making the total reactor height three times the height of the regolith bed.

Recent fluidization experiments not yet completed showed good fluidization achieved with a pulsing flow of hydrogen instead of a constant flow. By injecting half the flow rate normally required for fluidization in pulses with equal on-off times, the injection velocity should be similar to that for the full flow on continuously and sufficient to provide good fluidization. While the hydrogen gas is introduced into the reactor in a pulsed manner, the reactor appears to provide a large enough plenum volume such that the flow becomes more steady-state within the chamber.

The transport disengagement height can therefore be much smaller as it is dependent on the velocity in the upper portion of the reactor. Lower total flow rates through the reactor will also benefit downstream components such as the water and gas cleanup subsystems that are sized based on total gas throughput.

To model the expected reaction rates for this type of mixing scheme, the well-stirred reactor option was used. Although this option was originally developed to model a reactor with a mechanical means to mix the gas and regolith, such as forced vibration or an internal auger, observations of the pulsed-flow tests appear to meet the basic premise of a well-stirred reactor. The well-stirred reactor option uses a specified hydrogen input flow rate and assumes that the gas is well-mixed with the regolith.

IV. Moisture Content

Because the hardware designers desire to limit the hydrogen flow rate to reduce the mass of the downstream components, the effects of varying the hydrogen flow rate into the reactor were investigated. As described in detail in ref. 11, the reaction equations are based on a shrinking core model. The model predicts, and experiments have validated, that reaction occurs quickly in the beginning of a batch where there is a large surface area exposed and the reaction is limited only by the equilibrium of the chemistry. Once the oxygen has been extracted from the easily accessible outer surface area of each particle, further extraction is slower as the process now becomes dominated by the diffusion of the hydrogen reactant into the particle's core and the water product back out. If the total hydrogen flow rate into the reactor is limited, it is possible to starve the initial surface reaction portion and prevent the conversion to water from reaching the equilibrium potential:

$$FeO + H_2 \Leftrightarrow Fe + H_2O \tag{2}$$

To understand the performance as a function of time and hydrogen flow rate, the conversion was calculated using the hydrogen reduction model and the JSC-1A simulant. While this simulant is low in ilmenite, it has an overall iron oxide content of 11.2 percent and may behave similarly to low-ilmenite soils such as those found in the lunar highlands during Apollo. This simulant also has been used the most in laboratory tests, and the data from these tests have been used to validate the model for this simulant.[11] For the moisture content analysis, the amount of regolith and the reactor diameter, pressure, and operating temperature were held constant at some typical values (Table I). With these inputs, the required hydrogen flow rate for a fully fluidized bed is 160 SLPM (0.119 gm/s).

Table I. Inputs for moisture analysis.

Parameter Name	Value	Units
Simulant	JSC-1A	
Sorted	no	
Ave Particle Size	93	microns
Reactor Option	Well-Stirred	
Reactor Inner Diam.	0.146	m
Reactor Pressure	25	psia
Reactor Temperature	1323	K
Regolith Quantity	12.5	kg
H_2 flow rate	40	SLPM
Model Used: HydrogenReductionModel v6.3		

Figure 1. Water product out of reactor for limited (well-stirred) and large (fluidized) hydrogen flow rates.

This was compared to a flow rate of 40 SLPM (0.056 gm/s) using the well-stirred reactor option, and the results for water flow rate out are shown in Fig. 1. The horizontal line for the well-stirred reactor option clearly indicates that the reactor is operating hydrogen-starved for most of the first hour of the batch. However, once all the oxygen from the particles' surface has been extracted and the reaction moves into the slower, diffusion-limited phase, the lower flow rate case quickly catches up in total conversion as shown in Fig. 2. Therefore, there should be no loss in total yield with lower hydrogen flow rates if the regolith is allowed sufficient time in the reactor. This assumes that sufficient mixing and heat transfer can be obtained either through pulsing or other mechanical methods.
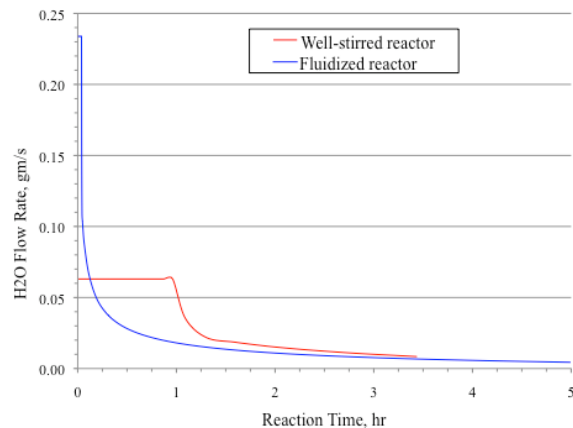
This type of analysis can also be used to investigate the effects of bringing hydrogen into the reactor with some amount of moisture already in it. For this analysis, reaction time was held constant at 2 hours and the fraction of moisture in the incoming hydrogen stream was varied until the conversion rate dropped to zero (Fig. 3). At a moisture content of 6 mole percent (36 mass percent) the conversion has dropped by approximately one-third, from 60 percent of maximum potential yield to 41 percent, and then drops sharply down to zero conversion for a moisture content just under 10 mole percent (50 mass percent).
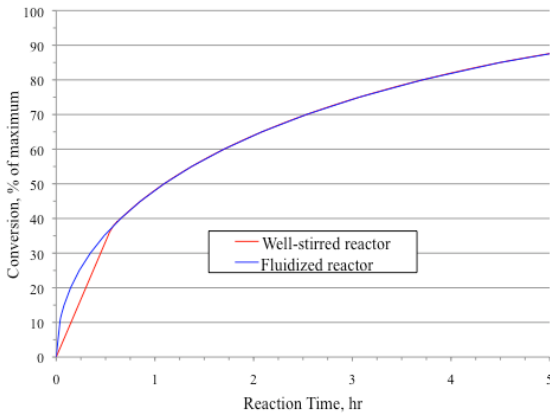
Figure 2. Effects on conversion potential with limited and large hydrogen flow rates.
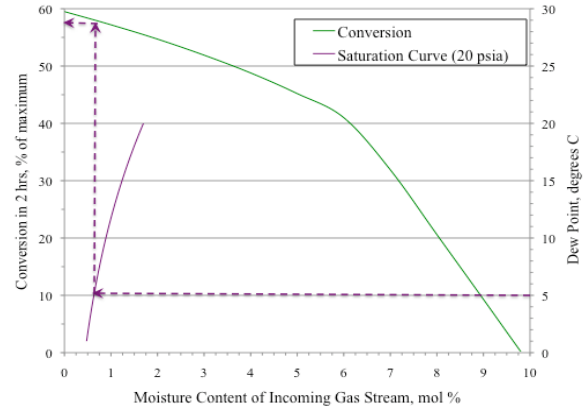
Figure 3. Reduction in conversion with increasing moisture content in hydrogen gas stream.

Figure 3 can also be used to understand how the operating temperature of the condenser will affect the conversion rate. A saturation curve is included with saturation pressure converted to mole fraction of water in the hydrogen stream assuming an operating pressure of 20 psia. Assuming the condenser is operating at 5 degrees C, for example, the moisture content is approximately 0.6 mole percent water which results in about a 2 percent drop in conversion for a 2-hour batch. Higher condenser operating temperatures or lower operating pressure will result in a higher moisture content going into the reactor and a larger reduction in conversion.

V. Heat-up and Reaction Time

The primary question for reactor operation is how much time should be allotted to processing each batch of regolith, and what should be the split between heat-up time and reaction time. Previous analysis showed that the percent conversion increases fairly quickly up to about 70 or 80 percent of the total potential, and significant additional time is required to gain the last 20 to 30 percent conversion. From an energy standpoint there is a point then where the amount of oxygen produced per energy invested begins to decline. For conditions in the previous work this point is between 55 and 65 percent conversion, which requires 3 to 5 hours of processing time.[8] This relationship was the starting point for the following evaluation of sensitivities to reactor geometry, number of reactors, and insulation effectiveness. Processing time refers to an entire batch process including filling a reactor, heating the regolith to operating temperature, extracting oxygen in the form of water, heat recuperation (if included), and emptying the reactor of the spent regolith.

A. Power and Energy

Power required to maintain temperature in the reactor during reaction is calculated by multiplying the heat flux out of the reactor times the reactor outer surface area. The heat flux is a function of the reactor temperature, reactor material, and insulation type and thermal properties. The loss through the top and bottom of the reactor is assumed to be the same heat flux as through the side walls as a first approximation. The incoming hydrogen is assumed to be partially pre-heated in a heat exchanger with the outgoing hydrogen, and the energy required to heat this small thermal mass the rest of the way to operating temperature is currently not included. The reaction energy is the power times the reaction time. It is this energy loss that will determine the point of diminishing returns in terms of oxygen still being extracted per energy investment.

Power required for heat-up is calculated from the mass of regolith in the reactor and its average specific heat capacity, assumed to be 750 J/kg – K. Added to this value are the power required to heat up the reactor walls and the power required to make up for heat loss through the reactor walls. Since heat loss is a concern during both

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operations, it is of interest to see how the parameters that affect heat loss, primarily the reactor dimensions and insulation, will affect the balance between heat-up and reaction times.

The hydrogen reduction model was first run as a fluidized bed with a constant diameter in the range being considered for the next generation reactor and for a range of total batch or processing times. The total processing time was divided evenly between heat-up and reaction time, and then the reaction time was reduced 15 percent to allow time for dumping the spent regolith and filling with new regolith. The insulation thickness was initially assumed to be very large to minimize the effects of the heat loss. The initial parameters are listed in Table II.

Table II. Initial inputs for heat-up and reaction time analysis.

Parameter Name	Value	Units
Oxygen Production	1000	kg/yr
Insulation Type	Zircar AXL	
Insulation Thickness	0.12	m
Gravity	9.18	m/s2
Simulant	JSC-1A	
Sorted	no	
Ave Particle	93	microns
Reactor Type	Fluidized	
Reactor Inner Diameter	0.146	m
Reactor Pressure	14.7	psia
Reactor Temperature	1323	K
Regolith Inlet Temperature	273	K
Model Used: HydrogenReductionModel v6.3		

As the total time per batch is increased, more regolith must be processed per batch, causing the reactor size to grow. As discussed previously, the total reactor height for a fluidized bed is approximately 3 times the bed height, so the fluidized bed option predicts unrealistically large reactor heights for long reaction times and a small fixed diameter. The tall, skinny reactor also has a large surface area, which results in a large heat loss during heat-up and reaction. Therefore, the fluidized bed option was re-run with the reactor diameter varied for each reaction time such that the height-to-diameter (H/D) ratio was roughly constant. H/D ratios of 6 and 2 were evaluated and compared to the constant diameter option.

Figure 4 shows the total heat-up and reaction energy per day and the variation in conversion percent for the different reactor dimensions as a function of reaction time. As seen in the earlier work, the conversion percent increases with longer batch times. This increases total yield, which in turn decreases the amount of regolith that must be processed per day. Therefore, as reaction time per batch increases, the daily heat-up energy decreases as less regolith is heated per day. However, longer reaction times are only possible in larger reactors that can process more regolith per batch. Larger reactors result in more surface area and therefore higher heat losses during reaction. So while heat-up energy decreases with longer reaction times, the reaction energy increases. For the case of a constant diameter reactor, the height increases nearly directly with the regolith quantity causing a sharp increase in heat loss during reaction. Holding the H/D ratio constant is a more efficient way to increase reactor volume to accommodate the additional regolith, and the increase in surface area and therefore heat loss is more modest in those cases. Figure 5 combines the heat-up and reaction energy to show the total daily energy as a function of reaction time. While the benefits of reducing total regolith processed per day thereby reducing the heat-up energy dominates the total energy calculation for the more realistic reactor shapes, the small-diameter reactor actually shows an increase in total energy with longer batch times as the heat loss during reaction begins to dominate after approximately 3 hours.
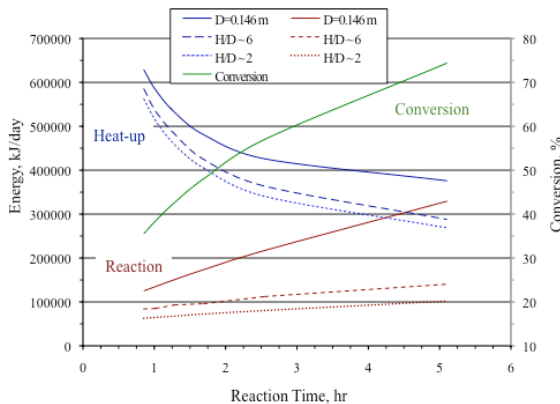

Figure 4. Heat-up and reaction energy for different reactor aspect ratios and reaction times for fluidized reactor.
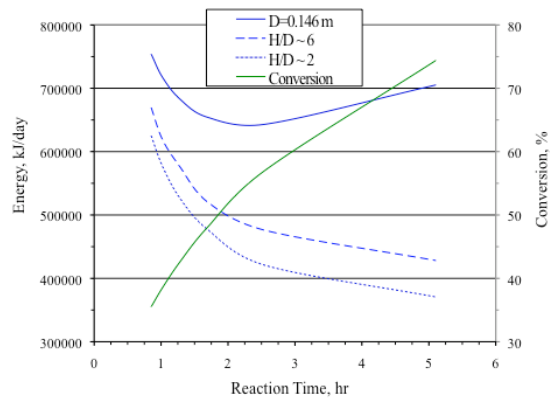

Figure 5. Total energy for different reactor aspect ratios and reaction time for fluidized reactor.

It can also be seen from Figs. 4 and 5 that the energy continues to decline as the reactor shape continues to get shorter and wider. For a fluidized bed, however, increasing diameter requires increasing hydrogen flow rate to fluidize, and these higher flow rates will affect the size and power consumption of downstream components such as the gas cleanup system, condenser, and compressors, as discussed previously.

Whereas controlling the H/D ratio is one method to control surface area and therefore minimize the heat loss, other methods also exist. As discussed previously, introducing the hydrogen into the reactor in a pulsed flow has shown promise of providing good mixing at much lower hydrogen flow rates. The well-stirred reactor option was used for this analysis and assumes the regolith and gas are well-mixed for a specified hydrogen flow rate. Since the pulse flow tests used equal on-off times for the hydrogen, a hydrogen flow rate of 75 SLPM was input, which is approximately half that calculated by the model for the fully fluidized case. All other variables were kept the same. The lower flow rates significantly reduced the transport disengagement height and therefore the surface area and heat loss term. Figure 6 shows the reduction in total energy from the fluidized option to the well-stirred option for an H/D ratio of 6. This reduction is approximately 19 percent at a reaction time of 2.5 hours and close to 25 percent for a 5-hour reaction time. It should be noted that it is likely that the pulse-mode of operation will also require higher total flow rates as diameter is increased as is the case for the fluidized bed. Therefore, an H/D ratio of 6 was used for the reactor aspect ratio in all remaining analyses discussed in this paper.
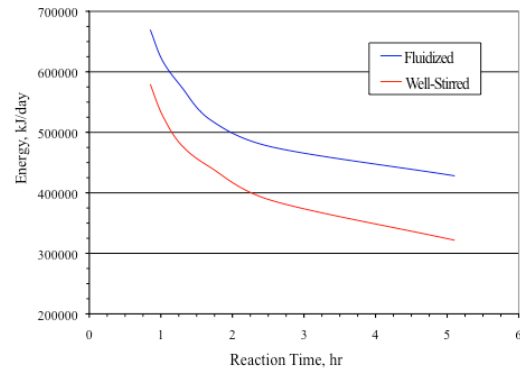

Figure 6. Effects of lower hydrogen flow rate on total energy for a reactor aspect ratio, H/D, of 6.

B. Three Reactors

Original analysis using the system models indicated that there was a significant reduction in overall power requirements by going from one to two reactors, but little additional gain for going to three reactors.[6] Two reactors best accommodated the two primary operations of the batch process, heat-up and reaction. Some recent concepts for recuperating the heat from the spent regolith before dumping include performing this heat transfer step within a multi-chambered reactor. This now introduces a third step to the process, that of heat recuperation, and it seems apparent that a third reactor will be needed to maintain near-continuous heat-up and reaction cycles. Although the driver for looking at three reactors is the assumption of some amount of heat recuperation, the analysis was first performed with three reactors assuming no heat recuperation as a baseline.

Three reactors for a 2-step process offer some flexibility in how to split the heat-up and reaction times. While one option is to split the time evenly as done with the two reactors, it is also of interest to investigate the trends if heat-up time is twice the reaction time or vice-versa. Figure 7 shows pictorially several options for splitting up
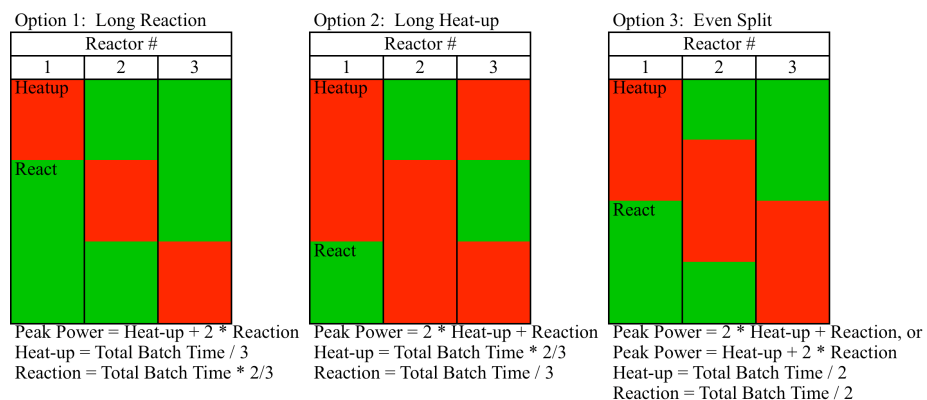

Figure 7. Operational options for three reactors without heat recuperation.

the total available process time and the equations for calculation of peak power for each option. The first two options allot either the same heat-up time or the same reaction time per batch as the two-reactor operation. For example, processing 12 batches per day in two reactors means each reactor processes 6 batches per day. That results in 4 hours per batch, with 2 hours for heat-up and 2 hours for reaction. Processing 12 batches per day in three reactors means each reactor processes 4 batches per day. That results in 6 hours per batch, with either 2 hours heat-

up and 4 hours reaction (Option 1: Long Reaction), 4 hours heat-up and 2 hours reaction (Option 2: Long Heat-up), or 3 hours for each (Option 3: Even Split). So the 'Long Reaction' option allots the same heat-up time with twice the reaction time, and the 'Long Heat-up' option allots the same reaction time with twice the heat-up time compared to the two-reactor operation.

In general, the trends of energy as a function of reaction time are similar for the three reactors as for the two reactors, with some variations in whether the energy continues to decline at long times or starts to increase (Fig. 8). Whereas it might be expected that three reactors are less energy efficient because of greater total surface area, there are many conditions where the total energy requirement for two and three reactors are very similar. Although the initial tendency may be to expect a reduction in peak power with an increase of the heat-up time, Fig. 9 shows that the peak power curves are nearly identical to the total energy curves in Fig. 8. So while the power required in any single reactor is reduced, it is taken up by the addition of a third reactor operating in parallel.
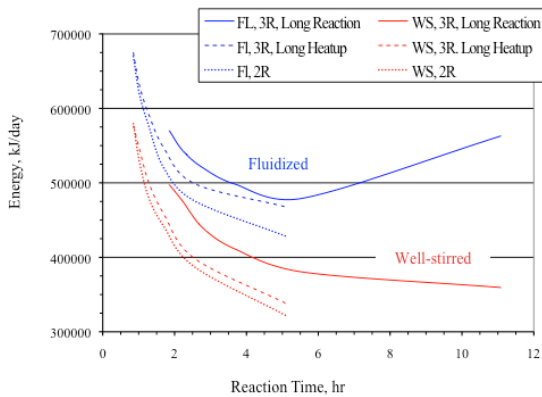

Figure 8. Energy comparison for two (2R) and three (3R) reactors for fluidized (FL) and well-stirred (WS) options.
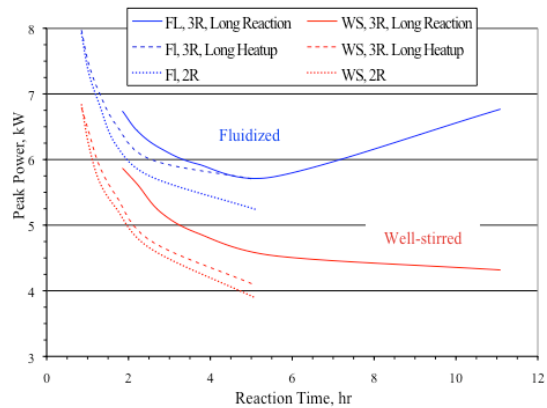

Figure 9. Peak power comparison for two (2R) and three (3R) reactors for fluidized (FL) and well-stirred (WS) options.

Finally, the total mass of the reactors is compared in Fig. 10 for the two- and three-reactor systems. For these comparisons the reactor mass includes the reactor walls (plus 30 percent margin), but does not include the insulation mass. It can be seen that while the two-reactor system has similar energy requirements to the three-reactor system with long heat-up times, the mass of the two-reactor system is similar to the three-reactor system with long reaction times. For comparisons to three reactors with heat recuperation in the next section, the three-reactor system with long heat-up times will be used as the lower energy option.

C. Three Reactors with Heat Recuperation

The problem with assessing the effects of adding a heat-recuperation operation to the reactor system is that the analytical calculation of how much heat can be transferred and how long it will take has proven to be difficult. The general concept assumed here is based on the current generation hardware design. After the hydrogen flow and therefore the reaction in a reactor have been stopped, a fresh load of regolith will be loaded into an annulus chamber surrounding the reaction chamber. After some amount of time, called the recuperation time, the spent regolith is dumped, and the pre-warmed regolith is transferred into the reaction chamber and electrically heated to reach the final operating temperature. With three reactors and three steps in the process, one obvious split is to allow each process an equal amount of time. Because the recuperation step is serving to heat up the regolith, this split could be expected to give similar results to the 'Long Heat-up' option in the earlier analysis without heat recuperation. A second option is to allot half of the time to
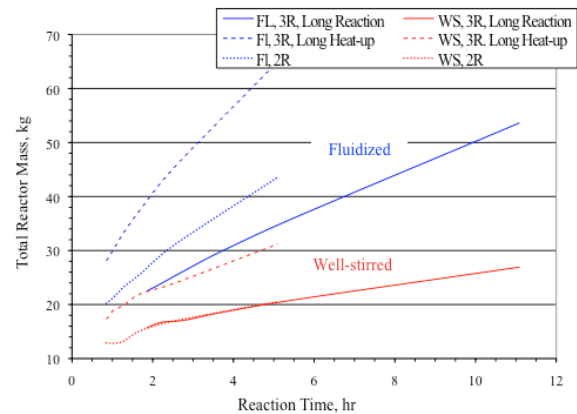

Figure 10. Reactor mass comparison for two (2R) and three (3R) reactors and fluidized (FL) and well-stirred (WS) options.

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the reaction step and split the remaining half between the recuperation and heat-up steps. These options are shown pictorially in Fig. 11 along with the equations for calculation of peak power.

Total daily energy as a function of reaction time is plotted in Fig. 12 for an H/D of 6, and equal times for heat-up, reaction, and recuperation (Option 4 in Fig. 11). Both fluidized and well-stirred reactor options and assumed heat recuperations of 30 and 50 percent are shown. With the recuperation concept described above, the maximum possible pre-heating of the fresh regolith would be 50 percent so this should be viewed as the theoretical limit for energy savings. Figure 13 shows the energy savings for 30 and 50 percent heat recuperation as compared to no heat recuperation. The savings is 20 to 25 percent for an assumption of 30 percent recovery, and 25 to 40 percent in the limit case of 50 percent recovery.
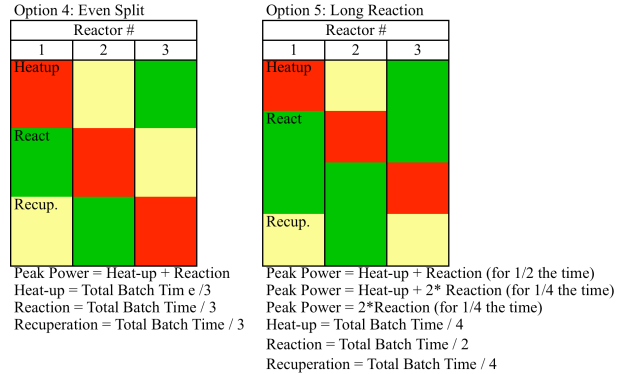

Peak Power = Heat-up + Reaction
Heat-up = Total Batch Tim e /3
Reaction = Total Batch Time / 3
Recuperation = Total Batch Time / 3

Peak Power = Heat-up + Reaction (for 1/2 the time)
Peak Power = Heat-up + 2* Reaction (for 1/4 the time)
Peak Power = 2*Reaction (for 1/4 the time)
Heat-up = Total Batch Time / 4
Reaction = Total Batch Time / 2
Recuperation = Total Batch Time / 4

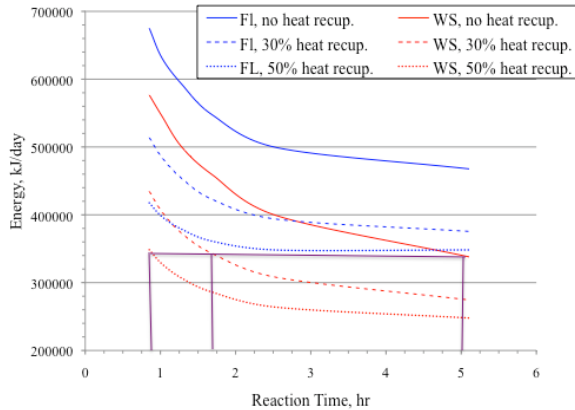**Figure 11. Operational options for three reactors with heat recuperation.**

Figure 12. Effects of heat recuperation on total energy for fluidized and well-stirred options.
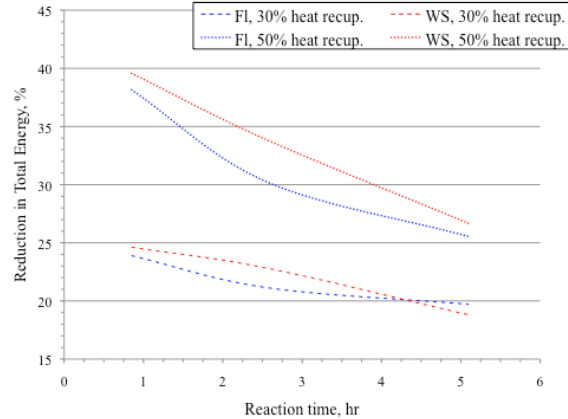

Figure 13. Energy savings from heat recuperation.

While Figs. 12 and 13 show that there is potential for significant energy reductions if heat recuperation proves successful, Fig. 12 also allows an interesting comparison between reaction time and pre-heating. For example, the daily energy required at just under 1-hour reaction time assuming 50 percent heat recuperation is the same as a 1.75-hour reaction time assuming 30 percent heat recuperation and a 5-hour reaction time assuming no heat recuperation. Increasing the reaction time or adding a recuperation outer chamber will both increase the mass of the reactors. The recuperation concept envisioned here will also add mass and operational complexity for components needed to perform the extra regolith transfer step. All of these factors must be considered when selecting the optimum reactor design and operating concept.

Figures 12 and 13 show energy comparisons for a three-reactor system where heat-up time, recuperation time, and reaction time are all equal. The second option where reaction time is allotted half of the total batch time (Option 5 in Fig. 11) was also evaluated and the results are plotted in Fig. 14 for the well-stirred reactor only, along with the results for the equal splits. This 'long reaction' option has similar, but slightly higher, energy trends as the 'equal split' option.

Finally, Fig. 15 shows the mass of all the reactor system options for the well-stirred reactors. While the model does not include a calculation for the mass of the reactors with a heat recuperation chamber, for a first approximation the calculated single chamber reactor mass was multiplied by two to account for the mass of the heat recuperation chamber. The mass for 30 percent and 50 percent heat recuperation are equal if all other parameters are held constant, so only the 50 percent heat recuperation curves are included in Fig. 15. In general, choices that favor reaction time over heat-up time will produce a higher yield, resulting in less regolith to process per day and therefore

lower reactor masses. Considering both Figs. 14 and 15 together, it is clear that selections for minimum energy will be opposite selections for minimum mass. Two or three reactors with no heat recuperation and short batch cycles (resulting in short reaction times per batch) will result in the lowest mass reactors and the highest energy requirements. Increasing the length of the batch cycle (resulting in long reaction times per batch), lengthening the heat-up time at the expense of the reaction time, and adding in a heat recuperation step will all decrease the energy requirement while increasing the reactor mass. The hardware designer must find the conditions that offer the best mix of low energy and low reactor system mass.
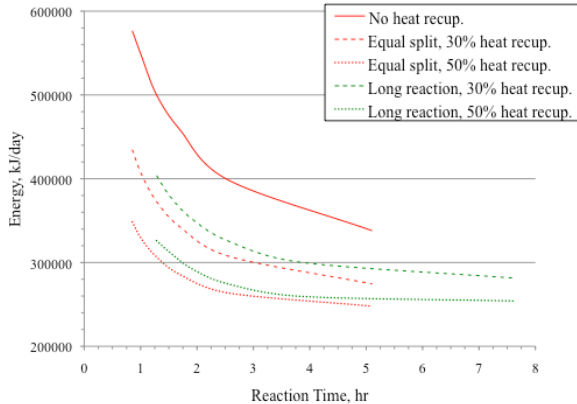

Figure 14. Comparison of effects of processing time on energy for a well-stirred, three-reactor system.
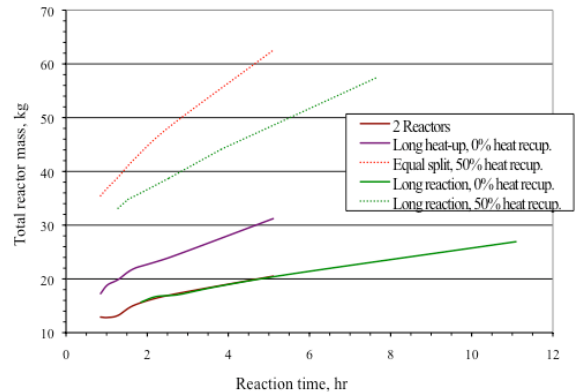

Figure 15. Comparison of reactor system mass for different operational options.

VI.   Sensitivities

In the preceding analysis many parameters were held constant while investigating the two- and three-reactor operations. Insulation thickness will affect the heat flux out of the reactor and therefore the total energy required. Operating pressure will affect the reaction rates and yield and therefore will also affect the total energy required. Some of the conditions examined above were reevaluated at other values of insulation and pressure to understand the sensitivities of the magnitude of energy required and also if these parameters may alter the trends exhibited and therefore guide the hardware designs in different directions.

A. Insulation Thickness

As discussed earlier, the heat loss out of the reactor affects energy and power required during both the heat-up and reaction portions of the batch process. If the insulation thickness is decreased, the heat flux and therefore the heat loss term will increase. It was anticipated that a significant change in the heat loss term could change the trends seen earlier, where longer reaction times resulted in an increased yield, reducing the total regolith processed per day as well as the energy required for heating. Figure 16 shows the daily energy required for a well-stirred reactor with increasing amounts of heat recuperation with a relatively small layer of insulation (0.0254 m). It is clear that while the energy required has increased 10 to 50 percent compared to the well-insulated case (Fig. 14) the trends of energy with time are very similar.
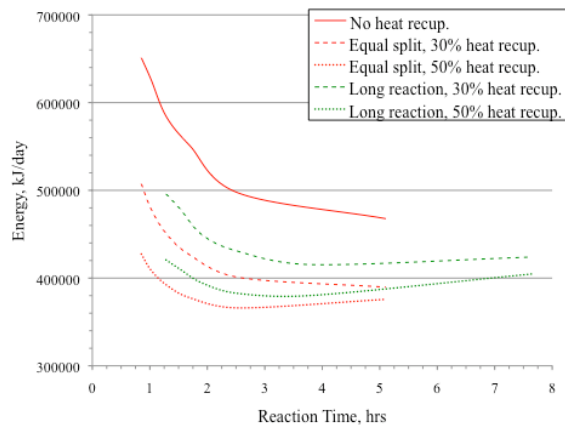

Figure 16. Energy for a well-stirred, three-reactor system with minimum reactor insulation.

B. Operating Pressure

The operating pressure in the reactor has a considerable effect on the reaction rates through the factor F described in ref. 11. This factor varies inversely with iron oxide content and particle size, and directly with the gas concentration in the reactor and the intra-particle gas

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diffusion coefficient. The pressure's primary effect is in the gas concentration in the reactor (mol/m^3, for example), so as pressure increases the F-factor and therefore the yield increases linearly. It should be noted, however, that this is primarily based on theory, and there has been very little test data generated at pressures other than 1 atm.

Figure 17 shows the improvement in yield for any given reaction time as the pressure is increased from 1 atm to 2.7 atm (101 MPa to 275 MPa). This translates directly into energy savings also shown in the figure. In addition to reducing energy requirements by 20 percent (at a 5-hr reaction time) to 35 percent (at a 0.85-hr reaction time), the increased reaction rates with increasing pressure also creates a flatter energy curve, especially for reaction times greater than 2 hours. This trend suggests that for the higher operating pressures reaction times need not be any greater than approximately 2 hours, which will keep the reactor mass down with only a small penalty in total energy.

Figure 18 shows the same curves for energy at the three pressures as in Fig. 17, and also includes the energy curves with heat recuperation at a pressure of 1 and 1.7 atm. This illuminates another trade that is available to the hardware designer: a trade-off between operating pressure and heat recuperation. For example, the energy required for the 3-reactor system operating at 1.7 atm with no heat recuperation is only slightly greater than the energy required for the system operating at 1 atm with 30 percent heat recuperation. Similarly, the energy required for a pressure of 2.7 atm and no heat recuperation, 1.7 atm with 30 percent heat recuperation, and 1 atm with 50 percent heat recuperation are all within 10 percent.
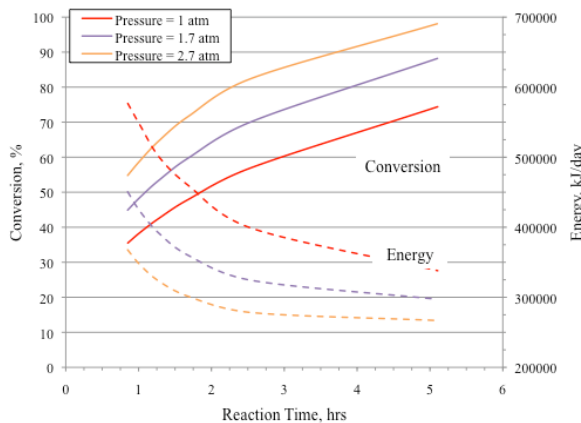

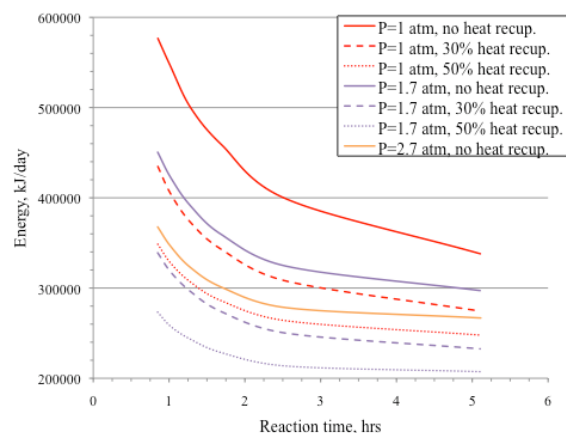**Figure 17. Improvement in conversion and energy with increasing reactor operating pressure.**

Figure 18. Comparison of methods for reducing total daily energy.

D. Other sensitivities

There are still other parameters that can affect the operation of the reactors that were not studied here. Reaction rates will increase with reactor temperature, both by increasing the equilibrium constant and thereby speeding up the chemistry-limited portion, and by increasing the diffusion coefficient and thereby speeding up the diffusion-limited portion. Smaller average particle sizes will also increase the reaction rate, as discussed in ref. 8. Smaller particles have a larger surface-to-volume mass fraction, thereby readily exposing more of the iron oxide to the faster equilibrium chemistry-driven portion of the reaction. Smaller particles also have a shorter diffusion characteristic length, thereby speeding up the diffusion-limited portion of the reaction as well. However, restricting particle size implies additional components that would be needed to first beneficiate the regolith, either through size improvement, mineral enrichment, or both. A complete study of these behaviors will be performed after models are written for these beneficiation components and included in the overall system balance.

VII. Conclusions

Reaction time, number of reactors, heat recuperation, heat loss, and operating pressure were all studied to understand the effects on the mass and energy requirements of a hydrogen reduction reactor system in an effort to guide the hardware designers for future prototype reactors. Longer reaction times provide a lower overall energy, except for reactors with high aspect ratios. However, longer reaction times per batch translate to fewer batches per day and therefore larger and heavier reactors. Three reactors with long heat-up times results in similar energy requirements as a two-reactor system with all other parameters the same. Three reactors with heat recuperation

results in energy reductions of 20 to 40 percent compared to a three-reactor system with no heat recuperation. Increasing operating pressure can provide similar energy reductions as heat recuperation for the same reaction times.

The hardware designers can use this new understanding of the behavior of two- and three-reactor systems with and without heat recuperation to guide the design of future prototype reactors.

Acknowledgments

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