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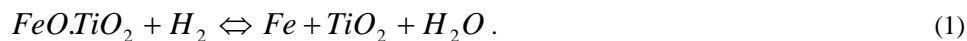
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**Abstract.** Lunar regolith will be used for a variety of purposes such as oxygen and propellant production and manufacture of various materials. The design and development of chemical conversion reactors for processing lunar regolith will require an understanding of the coupling among the chemical, mass and energy transport processes occurring at the length and time scales of the overall reactor with those occurring at the corresponding scales of the regolith particles. To this end, a coupled transport model is developed using, as an example, the reduction of ilmenite-containing regolith by a continuous flow of hydrogen in a flow-through reactor. The ilmenite conversion occurs on the surface and within the regolith particles. As the ilmenite reduction proceeds, the hydrogen in the reactor is consumed, and this, in turn, affects the conversion rate of the ilmenite in the particles. Several important quantities are identified as a result of the analysis. Reactor scale parameters include the void fraction (i.e., the fraction of the reactor volume not occupied by the regolith particles) and the residence time of hydrogen in the reactor. Particle scale quantities include the time for hydrogen to diffuse into the pores of the regolith particles and the chemical reaction time. The paper investigates the relationships between these quantities and their impact on the regolith conversion. Application of the model to various chemical reactor types, such as fluidized-bed, packed-bed, and rotary-bed configurations, are discussed.

## INTRODUCTION

Lunar mare basalts containing oxygen include olivine, ilmenite, and pyroxene (Heiken et al., 1991). Energy has to be supplied to remove the oxygen, i.e., the associated chemical reactions are endothermic. Free energy considerations show that the iron containing minerals require the least energy input for this purpose (Taylor and Carrier, 1992). Various technologies have been proposed for the chemical conversion such as ilmenite reduction by hydrogen, molten electrolysis, and carbothermal reduction using methane (McKay and Allen, 1996, Rice et al., 1997). The reduction processes involve solid-gas reactions. Such systems are well developed for earth applications but mainly for the purpose of metal extraction as opposed to water vapor and oxygen extraction for lunar applications. In addition, in the lunar context, the reactor must interface with the other sub-system processes such as upstream regolith extraction and beneficiation, and downstream electrolysis and phase separation in a way that establishes the most favorable balance between efficiency, robustness, and equivalent system mass. A need exists, therefore, to establish an analytical framework to couple these sub-systems together. The building blocks of this framework are the individual sub-system models. This paper discusses the development of a generalized analytical model of the chemical reactor sub-system.

While the developed methodology should be applicable to different gas-solid reactors, only the reduction of ilmenite by hydrogen will be considered here. Ilmenite is a major component of titanium-rich mare basalts. The overall gas-solid reaction considered is given by:



The formed water is electrolyzed in the electrolyzer subsystem to produce oxygen. This electrolysis process is not considered in the model development here.

The temperature of the reaction is one of the important parameters of the process. Ilmenite is just one constituent of mare basalt and it cannot be assumed that regolith beneficiation (e.g., in this case, removal of the non-ilmenite components) will be carried out prior to the reactor processes. The sintering and melting temperature of the unbeneficiated regolith is noted to be in the range of 1370-1670 K (Chambers, 1995, McKay and Allen, 1996). However, hydrogen reduction has been found to be effective at lower temperatures also, e.g., in the range of 970-1270 K (Yoshida et al., 2000). Therefore, while three-phase (gas-liquid-solid) reactors for hydrogen reduction may be applicable at post-melt temperatures, these are not considered here and attention is restricted to gas-solid interactions.

The equilibrium characteristics of the reduction reaction have been studied to some extent. An expression for the equilibrium constant as a function of the reaction temperature alone has been provided (William and Erstfeld, 1979):

$$k = 10^{(-2126.1/T + 0.6439)}. \quad (2)$$

More recently, computational studies have suggested a pressure dependence of the equilibrium constant (Altenberg et al., 1993), but the pressure sensitivity has been found to be much less than the temperature sensitivity. This is reasonable since gas phase moles are conserved in the reaction. The reaction rate and chemical kinetics of the reduction process appear to be much less studied. There is consensus that the reaction rate is of Arrhenius type and an activation energy for the forward reaction has been estimated (Butler et al., 2001) as 18.8 kcal/mole. As noted earlier, the conversion is endothermic and energy needed for conversion,  $\Delta H$ , has been estimated to be 11kJ/mol (Yoshida et al., 2000).

According to Eq. (2), the equilibrium constant for the temperature range of interest is of the order of 0.1. This suggests that substantial excess hydrogen beyond the stoichiometric value is needed to completely reduce the regolith. Therefore, a closed system where a batch of regolith and a fixed amount of hydrogen are placed in a vessel and allowed to react is not practical because of the large volume of hydrogen required to provide the needed oxygen for realistic regolith batch amounts. Thus, an open system where a batch of regolith is treated with flowing hydrogen is considered here.

The conversion process may be modeled in terms of the following overall steps: (i) inflow of hydrogen into the regolith containing reactor, (ii) reaction of hydrogen with the ilmenite portion of the regolith, and (iii) outflow of left-over hydrogen and produced water vapor. Step (ii) is the gas-solid reaction step which is the key to the conversion. Results of regolith particulate analysis conducted on Apollo-returned samples (McKay and Allen, 1996) suggest that the particles are not completely solid but have some porosity that would enable gases to diffuse into the particles, i.e., the FeO portion can be essentially completely converted with the reduced iron remaining behind in the particulates. These observations support utilization of a "shrinking core" diffusion-reaction model for the gas-solid reduction process (Levenspiel, 1998). This model must then be coupled with the inflow/outflow of gases to complete the reactor sub-system model. The chemical reactor analysis is carried out in the next section which is followed by a discussion of the obtained results.

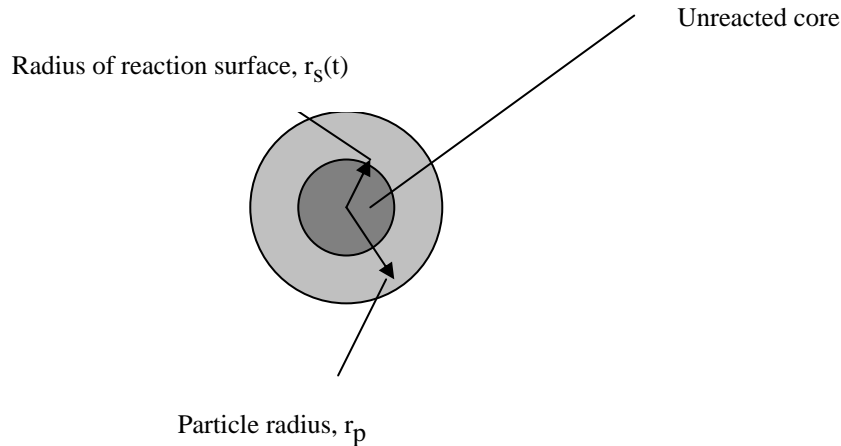
## MODEL DEVELOPMENT

In the first sub-section below, the shrinking core model for the hydrogen-regolith reaction is obtained. Shrinking core analyses in the literature generally assume an irreversible (forward only) reaction proceeding to completion. This assumption is mostly valid for cases where the equilibrium constant is large so that the gaseous reactant is almost all consumed at the reaction site. Here, the equilibrium constant according to Eq. (1) is of the order of 0.1 so that the amount of hydrogen must be well in excess of stoichiometric values for complete conversion of the regolith. Therefore, in general, both the forward and backward reactions must be considered. The regolith will also have a particle size distribution. Here, for simplicity, the regolith will be assumed to be comprised of identical spherical particles. Relaxation of this assumption is straightforward at the expense of increased book-keeping, but it does not change the qualitative features of the analysis. As the hydrogen flows through the regolith bed, because of depletion due to reaction, the concentration of hydrogen at the exterior surface of a particle will depend upon its location in the

reactor. This essentially is the coupling between the reactor flow and the gas-regolith reaction and is considered in the second sub-section below. Finally, the obtained solutions are assessed for applicability to different reactor types such as fluidized bed, packed bed, and rotary bed.

### Intra-Particle Gas-Regolith Reaction Analysis

The shrinking core model as envisioned here is schematically depicted in Fig. 1. Conversion proceeds from the exterior particle surface inward. As the reaction progresses into the interior of the particle, the reactant and product gases must diffuse through the particle matrix structure formed after the conversion.



**FIGURE 1.** Shrinking Core Model Configuration

The diffusion of hydrogen in the particle interior between  $r_p$  and  $r_s$  is considered. Assuming quasi-steady behavior, and an effective diffusion coefficient,  $D$ , for the gases in the interior particle matrix, the concentration,  $c$ , of hydrogen varies according to:

$$\frac{\partial}{\partial r} \left( r^2 D \frac{\partial c}{\partial r} \right) = 0 \quad . \quad (3)$$

Boundary conditions for  $c$  have to be provided at the core (reaction) surface radius,  $r_s$ , and at the exterior particle radius,  $r_p$ . Note that the particle typically preserves its original (unreacted) size even during the reaction process as the main constituents (i.e., the non-ilmenite portion) are largely unaffected.

At the core radius, let the concentration of hydrogen be  $c_s$ . The value of  $c$  at the particle radius is denoted by  $c_x$  where  $x$  refers to the location of the particle along the flow direction in the reactor. In terms of  $c_s$  and  $c_x$ , the solution of Eq. (3) yields:

$$Dc = \frac{D[c_s - c_x]}{[1/r_p - 1/r_s]} [1/r_p - 1/r] + Dc_x \quad . \quad (4)$$

The flux of hydrogen at the reaction surface may be obtained from the above equation to be:

$$D \frac{\partial c}{\partial r} \Big|_{r_s} = \frac{1}{r_s^2} D \frac{[c_s - c_x]}{[1/r_p - 1/r_s]} . \quad (5)$$

This hydrogen flux is related to the conversion of FeO at the reaction surface. With  $\rho_a$  being the molar concentration of FeO in the unreacted particle, the conversion of FeO by the flux of hydrogen is given by:

$$\frac{d}{dt} \frac{4}{3} \rho_a \pi r_s^3 = -4\pi r_s^2 D \frac{\partial c}{\partial r} \Big|_{r_s} . \quad (6)$$

Using the value of  $D(dc/dr)_{r_s}$  from Eq. (5) and solving for  $r_s$  yields:

$$3[1 - \alpha]^{2/3} - 2[1 - \alpha] - 1 = -\frac{6D[c_x - c_s]t}{\rho_a r_p^2} , \quad (7)$$

where  $\alpha$  is defined as:

$$\alpha = 1 - \frac{r_s^3}{r_p^3} . \quad (8)$$

Equation (7) is the shrinking core result in terms of the hydrogen concentration at the reaction surface and the overall particle surface. For the classical case of an irreversible reaction with all of the hydrogen being consumed at the reaction surface, the value of  $c_s$  above would be zero, while this is not the case here. In the next section, a description for  $c_x$  is provided and the connection between  $c_x$  and  $c_s$  is discussed.

### Reactor Bulk Flow Analysis

It is assumed that the regolith particles form a bed in the reactor. The packing of the particles is characterized by the linear loading,  $N/L$ , of the particles. For example, the loading for a packed bed will be greater than that for a fluidized bed. It is assumed that the gas flow through the bed is characterized by a bulk flow velocity,  $u$  and the species (i.e., hydrogen or water) concentration is a function of only the distance along the bed length,  $x$ . The hydrogen concentration,  $c_x$ , is a function of  $x$  due to depletion by the reaction. Neglecting inter-particle gas diffusion in the bulk flow, the convection of hydrogen is related to its depletion by reaction in the following manner:

$$\pi R_r^2 u \frac{\partial c_x}{\partial x} = 4\pi r_s^2 D \left( \frac{\partial c}{\partial r} \right)_{r_s} \frac{N}{L} . \quad (9)$$

Upon using the results from the previous section for  $(dc/dr)_{r_s}$  and incorporating the shrinking core result from Eq. (7), the following equation is obtained for  $c_x$ :

$$R_r^2 u \frac{\partial c_x}{\partial x} = -4D[c_x - c_s] \frac{N}{L} r_p \frac{[1 - \alpha]^{1/3}}{[1 - (1 - \alpha)^{1/3}]} . \quad (10)$$

This may be rewritten in the following form:

$$\frac{\partial c}{[c_x - c_s]} = -3 \left( 1 - \frac{V_{void}}{V_{bed}} \right) \left( \frac{D}{r_p^2} \right) \frac{[1 - \alpha]^{1/3}}{[1 - (1 - \alpha)^{1/3}]} \frac{\partial x}{u} . \quad (11)$$



The required boundary value for  $c_x$  at the inlet is:

$$c_x(x=0) = c_0, \quad (12)$$

where  $c_0$  is the concentration of hydrogen at the reactor inlet, i.e., the value of  $c_x$  at  $x=0$ .

It may be noted that the factor  $D/r_p^2$  is the inverse of the intra-particle diffusion time,  $t_D$ , and the factor  $V_{\text{void}}/V_{\text{bed}}$  is the void fraction in the bed (i.e., the volume not occupied by particles). The factor  $dx/u$  represents the residence time of the gases in an axial slice  $dx$  of the regolith bed. Correspondingly, a bed residence time,  $t_R$ , may be identified by the factor  $L/u$  where  $L$  is the length of the regolith bed.

The factor  $[c_x - c_s]$  appears in both the shrinking core result and the bulk flow analysis. For an inwardly directed diffusive flux of hydrogen to exist within the reacted portion of the particle matrix,  $[c_x - c_s]$  must be greater than zero. The form of this factor will depend upon the relationship between the diffusion time  $t_D$  and a chemical reaction time,  $t_c$ . This reaction time is related to the instantaneous forward and backward reaction rates of the hydrogen reduction reaction (Eq. (1)). Different cases may be envisioned such as:

(i)  $t_D \gg t_c$  : The rate of gas diffusion in the particles is much slower than the chemical reaction. In this case, the processes are intra-particle diffusion controlled, and the chemical reaction may be assumed to be in equilibrium.

(ii)  $t_c \gg t_D$ : The rate of chemical conversion is much slower than the intra-particle gas diffusion. In this case, the processes are reaction controlled.

(iii)  $t_c \sim t_D$ : Both the gas diffusion rate and chemical reaction rates are of similar magnitude, and need to be accounted for.

In this paper, attention is primarily focused on the methodology for case (i). The methodology for the other two cases is somewhat more complex and will be considered in future work.

Chemical equilibrium at the reaction surface implies that the local number of moles of water and hydrogen are related according to:

$$c_{1s} = kc_s, \quad (13)$$

where  $c_{1s}$  represents the molar concentration of water at the reaction surface. The sum of the molar concentrations of hydrogen and water (i.e., the overall molar concentration) at the reaction surface is, therefore,  $(1+k)c_s$ . The reduction reaction (1) results in no changes to the number of moles in the gas phase. It is therefore assumed that the overall molar concentration at all points in the flow/reaction domain is constant. This is a reasonable assumption when the variation of the thermodynamic pressure in the reactor bed is negligible. With the understanding that the inlet flow to the reactor is entirely composed of hydrogen at concentration  $c_0$ , the following relationship is obtained:

$$c_s = \frac{c_0}{(1+k)}. \quad (14)$$

Thus, Equations (7) and (11) provide two simultaneous equations for  $c_x$  and  $\alpha$  as functions of time,  $t$ . After considerable manipulation, the solution for  $\alpha$  may be written in the following form:

$$-4 \ln \left[ \frac{1 - (1 - \alpha)^{1/3}}{1 - (1 - \alpha_0)^{1/3}} \right] + \ln \left[ \frac{2(1 - \alpha)^{1/3} + 1}{2(1 - \alpha_0)^{1/3} + 1} \right] = 3(1 - \varepsilon) \frac{D}{r_p^2 u} x, \quad (15)$$

where the void fraction is denoted by  $\varepsilon$ , and  $\alpha_0$  is the value of  $\alpha$  at  $x=0$  and is given from Eq.(7) by:

$$3[1 - \alpha_0]^{2/3} - 2[1 - \alpha_0] - 1 = -\frac{6D[c_0 - c_s]t}{\rho_a r_p^2}. \quad (16)$$

Since  $k$  is of the order of 0.1 as noted earlier, only about 10% of the incoming hydrogen can, at most, be converted to water. As a reasonable first approximation, therefore, it may be assumed that  $\alpha$  is independent of  $x$ , i.e., all particles in the reactor are being consumed at the same rate. In this case, a closed form solution for  $c_x$  at the end of the reactor bed can be readily obtained by integrating Eq. (11) between  $x=0$  to  $x=L$ . The solution may be shown to be:

$$c(L) = \frac{c_0}{(1+k)} \left\{ 1 + k \exp\left[-3(1-\varepsilon)\left(\frac{D}{r_p^2}\right) \frac{[1-\alpha]^{1/3}}{[1-(1-\alpha)^{1/3}]} \frac{L}{u}\right] \right\}. \quad (17)$$

Correspondingly, the molar water concentration at the outlet is:

$$c_1(L) = \left(\frac{k}{1+k}\right)c_0 \left\{ 1 - k \exp\left[-3(1-\varepsilon)\left(\frac{D}{r_p^2}\right) \frac{[1-\alpha]^{1/3}}{[1-(1-\alpha)^{1/3}]} \frac{L}{u}\right] \right\}. \quad (18)$$

### Application to Different Reactor Types

The developed model may be applied to different reactor types and, as examples, three common types of configurations are considered below. It may be noted that the main reason the model is applicable to these reactors is that the regolith conversion is determined largely by diffusional processes occurring within individual particles which are largely independent of the bulk flow.

#### *Fluidized-Bed Reactor*

In a fluidized bed, the void fraction and flow velocity are coupled. The coupling is described in terms of experimental and/or analytical correlations (McCabe et al 2001). For example, for incipient fluidization in the viscous flow regime, the fluid velocity is related to the void fraction by:

$$u_f = \frac{(\rho_s - \rho_g)}{37.5\mu} g r_p^2 \frac{\varepsilon^3}{1-\varepsilon}. \quad (19)$$

Generally, the flow velocity,  $u$ , is chosen to be between the incipient fluidization velocity and the particle settling velocity,  $u_s$ :

$$u_s = \frac{(\rho_s - \rho_g)}{4.5\mu} g r_p^2. \quad (20)$$

Equations (17) and (18) may be utilized once  $u$  and  $\varepsilon$  are fixed.

#### *Packed-Bed Reactor*

In this type of reactor, the particle bed is generally constrained physically within a given volume. In conjunction with the regolith volume, this provides the void fraction. The flow velocity may be picked independently of the void fraction; however, excessive pressure drop may limit its value.

### Rotary-Bed Reactor

In rotary-bed reactors, the regolith bed undergoes a rotational motion. This may be implemented, for example, by rotor vanes within the reactor or by rotating the reactor vessel about its axis. Depending upon the intensity of the mixing, the reactor may be characterized as “weakly-stirred”, “moderately-stirred”, or “well-stirred”. These characterizations refer to how well the mixing smears out the average spatial gradients in the gas species concentrations and the particle conversion,  $\alpha$ . The weakly-stirred case maintains the spatial gradients and may be described by the procedure considered earlier, i.e., by Eqs. (15) - (18). In the well-stirred reactor, both the gas species concentrations and  $\alpha$  are independent of location. The value of  $c_X$  may then be identified with  $c(L)$  and the solution of Eq. (11) in conjunction with Eqs. (12) and (14) yields:

$$c(L) = \frac{c_0}{1+k} \left\{ 1 + \frac{k}{[1 + 3(1-\varepsilon)\left(\frac{D}{r_p^2}\right) \frac{[1-\alpha]^{1/3}}{[1-(1-\alpha)^{1/3}]} \frac{L}{u}]} \right\}, \quad (21)$$

and, correspondingly,

$$c_1(L) = \frac{kc_0}{1+k} \left\{ 1 - \frac{1}{[1 + 3(1-\varepsilon)\left(\frac{D}{r_p^2}\right) \frac{[1-\alpha]^{1/3}}{[1-(1-\alpha)^{1/3}]} \frac{L}{u}]} \right\}. \quad (22)$$

The equation for  $\alpha$  is obtained by substituting Eq. (21) for  $c_X$  in Eq. (7).

In the “moderately-stirred” case, spatial gradients exist in the gas phase concentration but are relatively weak in the particle conversion  $\alpha$ . In this case, utilizing a spatial average between  $x = 0$  and  $x = L$  for  $c_X$  yields the following equation for the spatial average of  $\alpha$ ,  $\langle \alpha \rangle$ :

$$3(1-\langle \alpha \rangle)^{2/3} - (1-\langle \alpha \rangle) - 1 = \frac{2t}{\rho_a} \frac{k}{(1+k)} \frac{1}{(1-\varepsilon)} \frac{u}{L} \frac{[1-(1-\langle \alpha \rangle)^{1/3}]}{(1-\langle \alpha \rangle)^{1/3}} X \left\{ \exp\left[-3(1-\varepsilon)\left(\frac{D}{r_p^2}\right) \frac{L}{u} \frac{(1-\langle \alpha \rangle)^{1/3}}{[1-(1-\langle \alpha \rangle)^{1/3}]} - 1\right] \right\}. \quad (23)$$

## RESULTS

The equations developed above serve to clarify several features of reactor performance. Important parameters in the solution are the diffusion time  $t_D$ , reactor residence time  $t_R$ , void fraction  $\varepsilon$ , and regolith particle conversion  $\alpha$ . The relationships between these parameters determine the output stream of the reactor.

### Diffusion Time-Residence Time Interaction

The ratio of the residence time to diffusion time is:

$$\frac{t_R}{t_D} = \left(\frac{L}{u}\right) \left(\frac{D}{r_p^2}\right). \quad (24)$$

As this ratio becomes large, Eq. (18) or (22) implies:

$$c_1(L) \rightarrow \frac{kc_0}{(1+k)} . \quad (25)$$

The above value of  $c_1(L)$  corresponds exactly to the equilibrium conversion for a batch system which is reasonable in this limit of large residence time. This value also represents the maximum possible molar conversion of hydrogen to water.

On the other hand as the ratio of residence time to diffusion time becomes small, i.e.,

$$\frac{t_R}{t_D} \rightarrow 0 , \quad (26)$$

then, Eq. (18) or (22) implies:

$$c_1(L) \rightarrow 0 \quad (27)$$

which indicates that no conversion takes place since the hydrogen rapidly sweeps past the regolith without time for intra-particle diffusion to occur.

### Regolith Particle Conversion $\alpha$

It may be shown that as  $\alpha$  tends to zero, the value of  $c_1(L)$  approaches the equilibrium conversion amount. This may be expected since this case represents the early stages of the conversion process where the reaction occurs on the surfaces of the regolith particles (i.e., there is no intra-particle diffusion involved). On the other hand, as  $\alpha$  tends to unity, the conversion is complete and consequently:

$$c_1(L) \rightarrow 0 . \quad (28)$$

Thus, molar conversion of hydrogen to water is highest during the early stages of the conversion and then decreases with decrease in the size of the unreacted particle core. Equivalently, the conversion decreases with time.

### Bed Void Fraction $\varepsilon$

The factor  $(1-\varepsilon)$  appearing in Eqs. (15) – (22) can be expressed as:

$$1 - \varepsilon = \frac{V_{regolith}}{V_{bed}} . \quad (29)$$

For fixed regolith volume, the above factor is changed by changing the volume of the bed. The relationship between bed volume, flow velocity, and residence time can become complex. However, for the special case of a cylindrical reactor of fixed radius, the effect of changing bed length while keeping velocity constant is cancelled by the corresponding change in residence time (see, for example, Eq. (18)).

### Temperature and Pressure

Temperature and pressure impact the conversion due to their influence on the equilibrium constant  $k$  and effective diffusion coefficient  $D$ . Equation (2) provides the dependence of the equilibrium constant on temperature. As temperature increases, the equilibrium conversion amount is increased. However, the temperature cannot be increased indefinitely and 1250-1300 K appears to be the maximum allowable feasible temperature range in order to avoid sintering of the regolith as noted in the introduction section.

The effective diffusion coefficient for the regolith has not been well characterized to date. However, one may expect that its temperature and pressure dependence will be similar to that of gas phase diffusion which is inversely proportional to pressure and directly proportional to temperature via typically a power law:

$$D = D_0 \left(\frac{P_0}{P}\right)^a \left(\frac{T}{T_0}\right)^b . \quad (30)$$

Thus, as pressure increases, the effective diffusion coefficient decreases implying an increase in the diffusion time  $t_D$ . On the other hand, as temperature increases, the diffusion coefficient also increases resulting in a decrease in the diffusion time.

### Endothermicity Effects

As noted in the introduction section, the conversion process is endothermic. Therefore, it is of interest to estimate the temperature drop of the regolith particles due to reaction. Let the regolith be heated up initially to temperature  $T_i$  and assume that gas and regolith are at the same temperature during the process. The temperature of the regolith as a function of the particle conversion  $\alpha$ , neglecting the gas phase effects, may be written from energy conservation as:

$$T(\alpha) = T_i - \frac{\rho_a \Delta H}{\rho_s C_{ps}} \alpha . \quad (31)$$

Typical values of  $\rho_a$ ,  $\rho_s$ ,  $C_{ps}$ , and  $\Delta H$  are  $5400 \text{ mol/m}^3$ ,  $3000 \text{ kg/m}^3$ ,  $750 \text{ J/(kgK)}$ , and  $11000 \text{ J/mol}$ . Using these values indicates a temperature drop of approximately 25 K for the regolith particles as a result of the chemical reaction. This is a negligible drop compared to an initial temperature of approximately 1300 K. Of course, this does not include possible temperature drop due to heat loss to the surroundings.

## CONCLUSIONS

An analytical model for a reactor for hydrogen reduction of ilmenite has been developed. The reactor outflow composition is derived by coupling a shrinking core regolith particle model with the bulk flow in the reactor. As a result, the interactions among the chemical, mass and energy transport processes occurring at the length and time scales of the overall reactor with those occurring at the corresponding scales of the regolith particles are obtained. For the case where gas diffusion inside the regolith particles is the controlling step, important parameters identified are the regolith bed void fraction, intra-particle gas diffusion time, and reactor residence time. These parameters are, in turn, related to flow velocities, reaction temperatures and pressures, as well as to the type of reactor. The maximum molar conversion of hydrogen to water is given by the equilibrium ratio and occurs when residence time is much greater than intra-particle diffusion time. Application of the model to fluidized bed, packed bed, and rotary bed configurations have been indicated.

## NOMENCLATURE

$\alpha$	particle conversion	$\mu$	gas viscosity ( $\text{Ns/m}^2$ )
$\langle \alpha \rangle$	spatial average of $\alpha$	a,b	numerical constants in effective diffusion coefficient expression in Eq. (19)
$\varepsilon$	void fraction in regolith bed	c	molar concentration of hydrogen in particle ( $\text{moles/m}^3$ )
$\rho_a$	molar concentration of ilmenite in regolith ( $\text{mol/m}^3$ )	$c_1$	molar concentration of water ( $\text{moles/m}^3$ )
$\rho_g$	gas density ( $\text{kg/m}^3$ )	$c_{1s}$	molar concentration of water at reaction surface ( $\text{moles/m}^3$ )
$\rho_s$	regolith density ( $\text{kg/m}^3$ )		

$c_s$	molar concentration of hydrogen at reaction surface (moles/m <sup>3</sup> )	$r_p$	regolith particle radius (m)
$c_x$	molar concentration of hydrogen at location x in reactor (moles/m <sup>3</sup> )	$r_s$	radius of reaction surface (m)
$c_0$	molar concentration of hydrogen at upstream end of regolith bed (moles/m <sup>3</sup> )	$R_r$	internal radius of reactor (m)
$C_{ps}$	specific heat of regolith (J/kg/K)	t	time (s)
D	effective gas diffusion coefficient (m <sup>2</sup> /s)	$t_c$	chemical time (s)
$D_0$	effective gas diffusion coefficient at reference temperature and pressure (m <sup>2</sup> /s)	$t_D$	intra-particle diffusion time (s)
$\Delta H$	endothermic heat of reaction (Joules/mole)	$t_R$	reactor residence time (s)
g	gravitational acceleration (m/s <sup>2</sup> )	T	temperature (K)
k	equilibrium constant	$T_i$	initial temperature of regolith at start of conversion (K)
L	length of regolith bed (m)	$T_0$	reference gas temperature (K)
N	number of regolith particles in the bed	u	velocity through reactor (m/s)
P	gas pressure (Pa)	$u_s$	incipient fluidization velocity (m/s)
$P_0$	reference gas pressure (Pa)	$V_{bed}$	volume of regolith bed (m <sup>3</sup> )
r	regolith particle radial coordinate (m)	$V_{void}$	void volume in regolith bed (m <sup>3</sup> )
		x	axial coordinate (m)

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<b>14. ABSTRACT</b> Lunar regolith will be used for a variety of purposes such as oxygen and propellant production and manufacture of various materials. The design and development of chemical conversion reactors for processing lunar regolith will require an understanding of the coupling among the chemical, mass and energy transport processes occurring at the length and time scales of the overall reactor with those occurring at the corresponding scales of the regolith particles. To this end, a coupled transport model is developed using, as an example, the reduction of ilmenite containing regolith by a continuous flow of hydrogen in a flow-through reactor. The ilmenite conversion occurs on the surface and within the regolith particles. As the ilmenite reduction proceeds, the hydrogen in the reactor is consumed, and this, in turn, affects the conversion rate of the ilmenite in the particles. Several important quantities are identified as a result of the analysis. Reactor scale parameters include the void fraction (i.e., the fraction of the reactor volume not occupied by the regolith particles) and the residence time of hydrogen in the reactor. Particle scale quantities include the time for hydrogen to diffuse into the pores of the regolith particles and the chemical reaction time. The paper investigates the relationships between these quantities and their impact on the regolith conversion. Application of the model to various chemical reactor types, such as fluidized-bed, packed-bed, and rotary-bed configurations, are discussed.					
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