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Identifying heat and mass transfer characteristics of metal hydride reactor during adsorption—Parameter analysis and numerical study

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ABSTRACT

The performance of a metal hydride reactor is highly dependent on its transport process. It is important to know how the transport process affects the performance, therefore two key parameters—heat transfer controlled reaction rate and mass transfer controlled reaction rate were introduced to explain this kind of effect. Moreover, a brief discussion about how to use the new parameters was given. In order to analyze the reactor performance and heat/mass transfer characteristics, a non-local thermal equilibrium model describing the actual adsorption process was formulated, and numerical simulations were carried out. Then the two parameters were applied for the same purpose. The result of the parameter analysis coincided well with that of the numerical simulation, which approved the validity of the two parameters in identifying heat and mass transfer characteristics of the metal hydride reactor.

1. Introduction

Metal hydride (MH) reactors play an important role in many industrial applications such as hydrogen storage, heat pump, thermal compression, etc. Research on the design and performance optimization of the reactors is essential for the efficient operation of corresponding systems, thus many authors are paying more and more attention in this aspect.

The configuration is the most important part in the design of a MH reactor. There are many types of reactors used in MH applications. The first type–tubular reactor (TR for short) is the earliest one that was developed and has been investigated extensively by researchers. According to where the alloy is packed, TR can be subdivided into two kinds: "inside the tube type" [1–5] and "outside the tube type" [6]. The former one is more popular, which is shown in Fig. 1 [3]. The inner filter tube is for the flow of hydrogen while the outer tube is for the flow of heat transfer medium; the layer between them packed with alloy or hydride is normally thin and some measures to enhance heat transfer can be taken. TR ("inside the tube type") generally features good sealing, high bearing pressure and guaranteed heat and mass transfer effect by using thin tubes. But its scaling-up encounters great difficulties because of the length restriction of the filter tube. TR in this article refers to "inside the tube type" hereafter.

The second type is the disc reactor (DR for short), flat in shape [7,8], in which hydrogen flows into or out of the reactor axially through the screen which covers the layer of alloy or hydride; meanwhile heat transfer is carried out by coil or other apparatus on the other side of the layer, as is shown in Fig. 2 [7]. It was once thought to be promising for obtaining a large heat transfer area and a fast reaction rate; however, only

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Nomenclature

A	area, m^2
A_s	specific surface area, m^2/m^3
C	specific heat capacity, J/(kg K)
E	activation energy, J/mol
h	heat transfer coefficient, $W/(m^2 K)$
ΔH	reaction heat, J/mol H_2
k	reaction rate constant, s^{-1}
K	permeability, m^2
$\dot{m}$	source term of reaction, $kg/(m^3 s)$
M_H	molar mass of hydrogen, kg/mol
P	pressure, bar $= 10^5$ Pa
Q	heat flow or hydrogen flow, W or mol/s
r	reaction rate, mol $H_2/(m^3 s)$
R_r	universal gas constant, J/(mol K)
t	time, s
T	temperature, K
U	gas velocity, m/s
V	volume, m^3
x	length in certain direction, m
X	reacted fraction
$\overline{X}$	average reacted fraction
ε	porosity
λ	thermal conductivity, W/(m K)
μ	dynamic viscosity, Pa s
ρ	density, kg/m^3

Subscripts

a	adsorption
b	boundary
CV	control volume
e	equilibrium
eff	effective
f	gas phase
g	actual atmosphere
h	heat transfer
hb	heat transfer boundary
in	inlet
ib	inertia boundary
m	mass transfer
mb	mass transfer boundary
s	solid phase
sf	between solid and gas phase
∞	heat transfer fluid

a small amount of alloy can be filled in this type of reactor. Furthermore, the bearing pressure, sealing and cumbersome heat transfer pipelines are all practical problems against its development and industrial application.

Lately, a new type of reactor—annulus–disc reactor (ADR for short) was proposed by Wang et al. [9], which is shown in Fig. 3. A configuration similar to shell and tube type heat exchanger was adopted, which aims at solving the problem of industrial scaling-up. Hydride is packed in the annulus–disc units of the reactor. Mass transfer occurs between alloy or hydride in the annulus–disc units and hydrogen in the tubes. Simultaneously heat transfer takes place between the annulus–disc units and the fluid outside them. The heat output of the system can be adjusted within a large range by changing the number of the annulus–disc units.

Many researches have been carried out on the performance analysis and optimization of the MH reactor after the configuration is determined. Usually average reaction rate was used as the main performance index, thus hereafter "performance" refers to average reaction rate. El Osery [10] presented a numerical study on tubular metal–hydrogen reactor packed with FeTi. 1-D mathematical model considering heat conduction and reaction kinetics was used in the work, and poor heat transfer was thought to be the main reason that caused the relatively low reaction rate. Mayer et al. [11] introduced mass transfer into the modeling of the transient process in cylindrical MH reactors, which included a TR and another type with the propagating of reaction in axial direction. The reaction fronts were recognized clearly in their

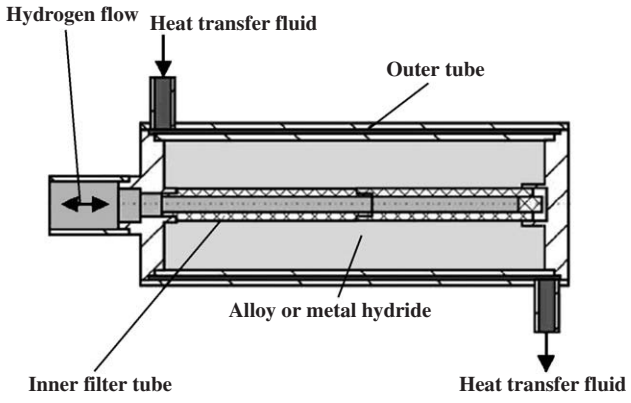

Fig. 1 – A schematic diagram of a TR.

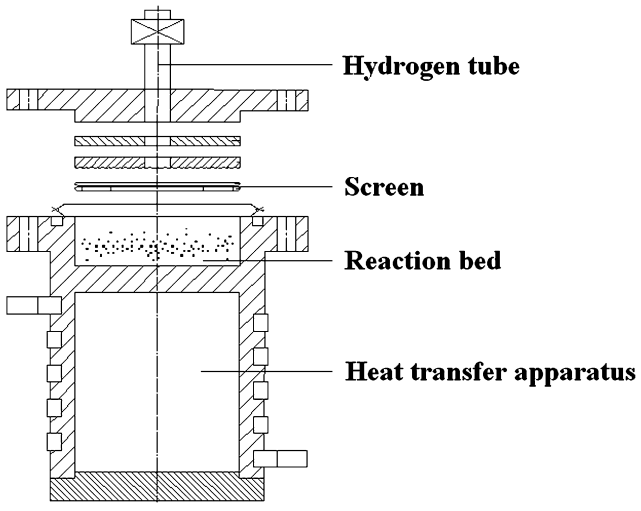

Fig. 2 – A schematic diagram of a DR.

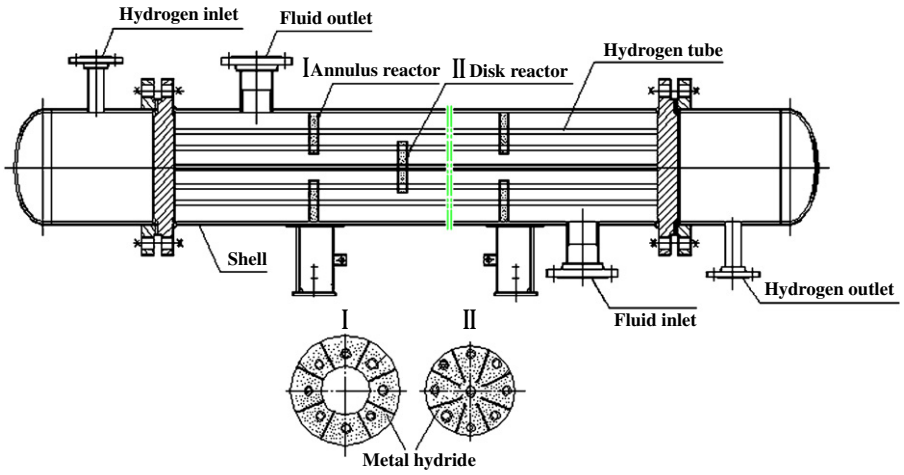

Fig. 3 – A schematic diagram and section view of an ADR.

simulation results, thus heat and mass transfer were found to be the key factors affecting the actual reaction rate in the reactor. Choi and Mills [12] proposed a 1-D model dealing with mass transfer by Darcy's law of porous media, and a disc reactor packed with $LaNi_{4.7}Al_{0.3}$ was taken for discussion. The authors concluded that mass transfer of hydrogen was not a rate limiting factor under the given conditions while thermal conductivity augmentation up to about 4 W/(m K) would lead to a significant improvement of the performance. Lately, Jemni and Ben Nasrallah [13,14] established a 2-D model considering the factors of heat and mass transfer of two phases in the reactor, and conducted detailed discussions for cylindrical reactors packed with $LaNi_5$ by numerical simulation. Their results indicated that the choice of proper geometry conditions was effective in improving the performance of the MH reactor, and the thermal conductivity augmentation to a certain extent could also enhance the performance. Moreover, the authors thought that the operation conditions such as inlet pressure of adsorption, temperature of heat transfer fluid were also the important factors affecting the performance of reactors. A 3-D model assuming thermal equilibrium was used in Mat et al.'s study for hydriding process in a cylindrical reactor [15]. Heat transfer coefficient and radius/height ratio must be chosen carefully since they were two important factors affecting the performance of the reactor significantly. A similar study on the adsorption process in a TR was carried out by Ha et al. [16], in which more factors were varied to examine their influences on the performance of the whole reactor. It showed that the heat transfer governed the process under the given conditions, thus a higher thermal conductivity, smaller bed diameter and the presence of fins would accelerate the process.

Obviously the studies mentioned above deepen our understanding about the characteristics of dynamic process in MH reactor and prove to be helpful in the design and optimization of a metal hydride (MH) reactor. Usually they are more qualitative than quantitative, more case-dependent than general, therefore the essential characteristics of the process needs to be further explored. In this paper, two parameters—heat transfer controlled reaction rate and mass transfer controlled reaction rate were proposed for this purpose, then a non-local thermal equilibrium model describing the dynamic process of the adsorption in the MH reactor was formulated and solved numerically. The usefulness of the two parameters was validated by the numerical simulation results under various conditions.

2. Parameters definition

To characterize the dynamic process in a MH reactor, it is necessary to define the limit of the reaction rate in the reactor. It was found by former researchers [10–16] that heat and mass transfer are critical factors affecting the actual reaction rate. Thus it is possible to relate the heat and mass transfer processes to the limit of reaction rate. Here a key and interesting observation shows that heat and mass transfer taking place in a MH reactor are mainly in one direction in most cases. For example, both heat and mass transfer proceed in radial direction for TR, and proceed in axial direction for DR. For ADR, heat transfer mainly proceeds in axial direction while mass transfer mainly proceeds in radial direction. Therefore, these processes can be simplified to the penetration of heat or hydrogen flow from heat transfer or mass transfer boundary to inertia boundary with zero flow rate, thus the limit of reaction rate set by heat or mass transfer is defined as below.

(1) The temperature gradient, the effective thermal conductivity of the reaction bed, operation conditions and geometry conditions correspond to a value of heat flow by Fourier's law, which can be written as

$$Q_{h1} = \lambda_{eff} \nabla T \cdot A_h. \quad (1)$$

Meanwhile reaction enthalpy, reaction rate and geometry conditions correspond to another heat flow, that is

$$Q_{h2} = r \cdot V \cdot \Delta H. \quad (2)$$

The maximum value of Q_{h1} can be used as the upper limit of the heat flow allowed by the transport conditions. Suppose

$Q_{h1} = Q_{h2}$, it is related to a certain value of reaction rate, namely a limit. Then a new question arises, i.e., under what conditions should Q_{h1} be calculated? Obviously a larger temperature difference implies a higher heat flow as well as a higher limit of reaction rate. While the temperature of heat transfer boundary T_{hb} is approximately fixed as the operation condition, the heat flow is maximized when the temperature of the inertia boundary T_{ib} reaches the equilibrium temperature which corresponds to the exerted pressure. In this way we get an estimation of the reaction rate subject to heat transfer conditions, namely heat transfer controlled reaction rate r_h, which is given by

$$r_h = \frac{\lambda_{eff}((T_{ib} - T_{hb})/\Delta x_h)A_h}{\Delta H \cdot V}. \quad (3)$$

(2) Similarly, the pressure gradient of the reaction bed, the physical properties such as permeability and viscosity, operation conditions and geometry conditions correspond to a value of hydrogen flow by Darcy's law and the state equation of ideal gas, as is shown below

$$\vec{U} = \frac{K}{\mu}\nabla P_f, \quad (4)$$

$$Q_{m_1} = \vec{U} A_m \cdot P_{mb}/(R_r T_{mb}). \quad (5)$$

Meanwhile reaction rate and geometry conditions correspond to another hydrogen flow, which is given as

$$Q_{m2} = r \cdot V. \quad (6)$$

First we should find out the maximum value of hydrogen flow set by mass transfer conditions. While the pressure of the mass transfer boundary P_{mb} is fixed as the operation condition, the hydrogen flow is maximized when the pressure of the inertia boundary P_{ib} is kept in equilibrium with the initial temperature of the reaction bed. The second parameter—mass transfer controlled reaction rate r_m is given as

$$r_m = \frac{K/\mu \cdot ((P_{mb} - P_{ib})/\Delta x_m) \cdot A_m \cdot P_{mb}/(R_r T_{mb})}{V}. \quad (7)$$

So how can the two parameters be used for the reactor design after their formulation? Firstly, their values indicate the actual reaction rate that a given reactor under certain conditions can achieve. When the values of the two parameters are calculated, the smaller one sets the more stringent limit of the reaction rate by transport processes. If it is lower than the reaction rate calculated by the essential kinetics, which is always the case, the value can be taken as a rough estimation of the actual reaction rate. Secondly, they are powerful tools for the design and optimization of MH reactor. By comparing the values of the two parameters, we get an idea about where the bottleneck of the performance lies, heat transfer or mass transfer? Then we can set about working on the enhancement of the process identified as the rate controlling step. Obviously, increase in values of the two parameters, especially the smaller one will loosen the restriction of transport conditions on the reaction process, thus improve the performance of the reactor. Therefore, the corresponding measures to change the value of the target parameter can be proposed, and their effects can also be evaluated by analyzing the two parameters. Sometimes the increase in the value of one parameter may result in the decrease in the value of the other, thus the effect on the performance is not straightforwardly given. We will discuss such a case later in the paper.

Some notations in using the defined parameters are explained here.

(1) Values of the two parameters resulting from the given formulas are in an average sense. It is obvious that the heat or mass flow determined by transport conditions is a summed or lumped value, while reaction cannot proceed at the same rate throughout the reactor. Actually, when the flow allowed by transport conditions is maximized, as is supposed in the formulation of the two parameters, the reaction ceases on the inertia boundary. Therefore, if the two parameters are needed to be compared with reaction rate of essential kinetics, the latter should be averaged concerning the whole reactor, thus a value of $\frac{1}{2}$ of the maximum reaction rate will be a simple estimation.
(2) $(T_{ib} - T_{hb})/\Delta x_h$ is used in Eq. (3) instead of the temperature gradient, also a similar simplification is applied to Eq. (7), which brings about error. However, it is found by further deduction that the values of simplified expressions are around half of those for accurate ones assuming uniform reaction and common geometry, therefore this can be used as a modification.
(3) Some approximations of variables are taken in the calculation of the parameters. For example, the temperature of heat transfer boundary is assumed to be constant, which is equal to the temperature of heat transfer media given as the operation condition, but obviously it is not the case. However, the approximation provides simplicity and has enough accuracy when the convective heat transfer coefficient is large, which is always guaranteed in practical applications. Furthermore, some variables such as P_{ib}, P_{mb} and T_{mb} in the formulas may vary during reaction, but estimation of their corresponding ranges is not very difficult, and approximation based on the estimation can be applied.

3. Dynamic process modeling

Simulation study of the MH reactor began very early. A well-accepted method has been established by several researchers' study [12,17,18], in which the flow and heat transfer theory of porous media is applied to describe the dynamic process in the reactor. With detailed differences between two phases considered, the non-local thermal equilibrium model for adsorption is used, as is shown below.

Mass equation for solid phase:

$$\frac{\partial((1-\varepsilon)\rho_s)}{\partial t} = \dot{m}. \quad (8)$$

Mass equation for gas phase:

$$\frac{\partial \varepsilon \rho_f}{\partial t} + \nabla(\rho_f \vec{U}) = -\dot{m}. \quad (9)$$

Energy equation for solid phase:

$$\frac{\partial((1-\varepsilon)\rho_s C_s T_s)}{\partial t} = \nabla((1-\varepsilon)\lambda_s \nabla T_s) + h_{sf} A_s (T_f - T_s) + \dot{m}(\Delta H/M_H + C_p T_f). \quad (10)$$

Energy equation for gas phase:

$$\frac{\partial(\varepsilon\rho_f C_p T_f)}{\partial t} + \nabla(\rho_f C_p \vec{U} T_f) = \nabla(\varepsilon\lambda_f \nabla T_f) + h_{sf} A_s (T_s - T_f) - \dot{m} C_p T_f \quad (11)$$

Momentum equation for gas phase takes the form of Darcy's law in Eq. (4).

Reaction kinetic equations for either adsorption or desorption vary with the type of alloy that was used. The widely applied alloy—$LaNi_5$ was taken for discussion in the article. Kinetic equation for adsorption is [13],

$$\dot{m} = k_a \exp\left(-\frac{E_a}{R_r T_s}\right) \ln\left(\frac{P_g}{P_e}\right)(1 - X). \quad (12)$$

P–C–T state equation recommended by Dhaou et al. [19] is used, where a_i are the polynomial coefficients

$$P_e = \sum_{i=0}^{7} a_i (X)^i \exp\left(\frac{\Delta H}{R_r}\left(\frac{1}{T_s} - \frac{1}{303}\right)\right). \quad (13)$$

The boundary conditions of MH reactors can be classified into three types, adiabatic wall (or symmetry boundary), heat transfer wall and mass transfer boundary, which are specified below.

Adiabatic wall (or symmetry boundary):

$$\frac{\partial T_s}{\partial x_h} = 0, \quad \frac{\partial T_f}{\partial x_h} = 0, \quad \frac{\partial P_g}{\partial x_m} = 0. \quad (14a)$$

Heat transfer wall:

$$(1-\varepsilon)\lambda_s \frac{\partial T_s}{\partial x_h} = h_s(T_s - T_\infty), \quad \varepsilon\lambda_f \frac{\partial T_f}{\partial x_h} = h_f(T_f - T_\infty), \quad \frac{\partial P_g}{\partial x_m} = 0. \quad (14b)$$

Mass transfer boundary:

$$\frac{\partial T_s}{\partial x_h} = 0, \quad T_f = T_{in}, \quad P_g = P_{in}. \quad (14c)$$

Boundary conditions of TR and DR can be easily obtained from Figs. 1 and 2. The virtual volume shown in Fig. 4 is used as a representative domain of the whole unit for ADR. In the 2-D cylindrical coordinates, boundary conditions of the reactors ("left" and "right" in axial direction, "top" and "bottom" in radial direction) are summarized in Table 1.

A fully implicit scheme based on the control volume method was used to discretize the governing equations, then line-by-line iterative method was used to solve the resulting algebraic equations. For TR, DR and ADR, 30×10, 10×50 and 10×58 grids were used, respectively, for simulation, and the time step was chosen to be 0.01s. Converge was achieved when error of T_s, T_f and P_g were lower than 10^{-3} K, 10^{-3} K and 10^{-6} bar, respectively.

4. Results and discussions

In the two parameters, many key factors affecting the performance of a MH reactor are taken into consideration, including the design dimensions, operation conditions, physical properties and configuration. The sequence of the discussion is as follows: TR was used to study the effect of variation in design dimensions and operation conditions on the performance of reactor, then performances for reactors of different configurations were compared. All the results were calculated, respectively, by numerical simulation and parameter analysis, and then comparison was made to testify the validity of newly introduced parameters. The performance of MH reactor was measured by average reaction rate, which was reflected by temporal changes of average reacted fraction defined in the following equation, $X(i,j)$ was the reacted fraction for the control volume (i,j):

$$\overline{X} = \frac{\sum_{i=1}^{m}\sum_{j=1}^{n} X(i,j) V_{CV}(i,j)}{\sum_{i=1}^{m}\sum_{j=1}^{n} V_{CV}(i,j)}. \quad (15)$$

The physical properties of the material (powders) and data in the simulation were listed in Table 2. When porous metallic hydride (PMH for short) compacts are considered, permeability, porosity and thermal conductivity of the solid phase are 10^{-14} m^2, 0.43 and 10 W/(m K) [20], respectively. The length, inner diameter and bed thickness of a TR are, respectively, 60, 40 and 20 mm. To guarantee the comparability, the thickness of DR and ADR are 20 mm too; the

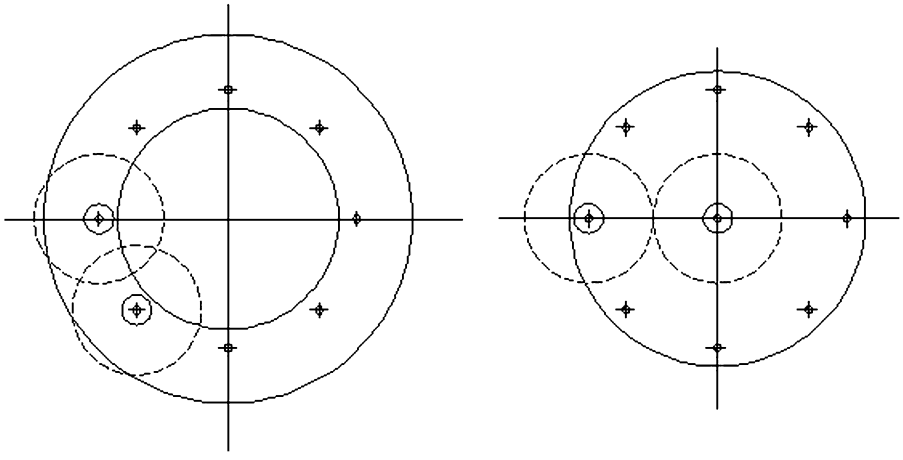

Fig. 4 – Virtual volume for computation in the annulus and disc units.

Table 1 – Boundary conditions for the three types of reactors

	Left	Right	Top	Bottom
TR	Adiabatic wall	Adiabatic wall	Mass transfer boundary	Heat transfer wall
DR	Mass transfer boundary	Heat transfer wall	Symmetry boundary	Adiabatic wall
ADR	Heat transfer wall	Symmetry boundary	Mass transfer boundary	Adiabatic wall

Table 2 – Physical properties of material (powders) and data used in the simulation

	Metal ($LaNi_5$)	Hydrogen
Density, ρ_s, kg/m^3	8400	–
Specific heat, C_p, J/Kg K	419	14 890
Thermal conductivity, λ, W/m K	2.4	0.16
Permeability, K, m^2	1.11×10^{-12}	–
Reaction enthalpy, ΔH, J/mol	3.1×10^4	–
Porosity, ε	0.50	–
Universal gas constant, R_r J/mol K	–	8.314

diameter of DR, the inner diameter and outer diameter of ADR virtual volume are 100, 60 and 350 mm, respectively. The temperature and reacted fraction of reaction bed are 293 K and 0.05, and equilibrium is assumed initially. The inlet pressure and temperature of hydrogen are 8 bar and 293 K, respectively. The temperature of heat transfer media is kept constant at 293 K.

Given the design and operation conditions, we can calculate the values of the two characteristic parameters. Take r_h of TR packed with powders, for example:

λ_{eff}, calculated according to equation $\lambda_{eff} = (1-\varepsilon)\lambda_s + \varepsilon\lambda_f$: 1.28 W/(m K),

T_{ib}, the temperature corresponds to 8 bar inlet pressure according to Eq. (13): 334.3 K,

T_{hb}, equals the temperature of heat transfer media: 293 K,

Δx_h, the radial thickness of bed: 20 mm,

A_h, the outer surface area of tube: 150.8 cm^2,

ΔH, reaction heat for $LaNi_5$: 31 000 J/mol H_2,

V, volume of tube: 226.2 cm^3.

By substituting the above specified values in Eq. (3), r_h of 5.684 mol H_2/(m^3 s) was obtained, as tabulated in Table 2, values of r_m can be calculated in the same way. Under the given conditions, the average reaction rate determined by essential kinetics according to Eq. (12) is around 200 mol H_2/(m^3 s), much bigger than the calculated value of r_h, so transport process, especially the heat transfer slows down the reaction. It shows that only simple algebraic procedure needs to be carried out in calculation of the characteristic parameters, then the parameters can be used for the design or optimization purpose with no complicated numerical simulation involved.

How do the variations in design dimensions affect the performance of a MH reactor? The answer can be found in Figs. 5 and 6. The inner radius R_{in} varies from 10 to 30 mm,

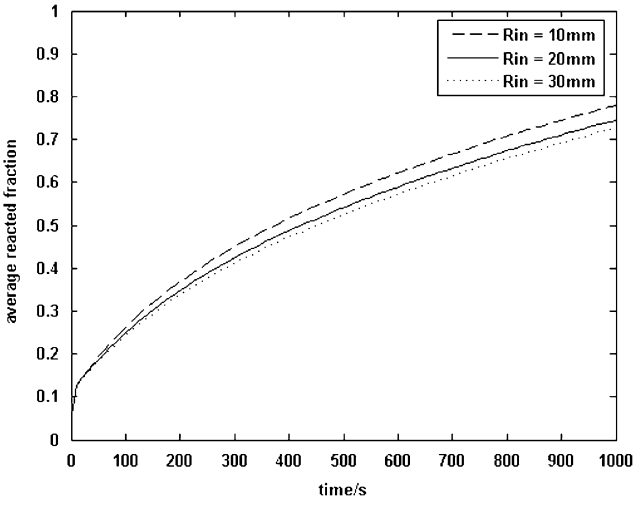

Fig. 5 – Performances for a TR with different inner radiuses.

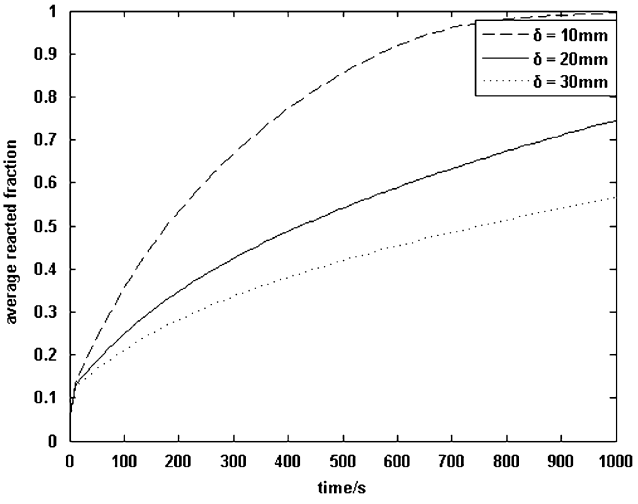

Fig. 6 – Performances for a TR with different thicknesses.

and the average reaction rate of reactor increases slightly with the decrease of R_{in}. The bed thickness δ is between 10 and 30 mm, the same trend similar to the discussion of R_{in} was observed for variation of δ, while the effect of δ on reactor performance is much more significant than that of R_{in}.

The effects of operation conditions on the performance of a reactor were shown in Figs. 7 and 8. The inlet pressure P_{in} varies from 6 to 10 bar while the temperature T_∞ of the heat transfer media varies from 283 to 303 K. The driving force of the reaction increases with the increase of P_{in} or the decrease

of T_∞, which favors the performance of the reactor, as can be seen in the two figures.

Then the sensitivity study of the reaction rate was carried out in another way. In Table 3 the values of the parameters under various given conditions were listed, and the smaller one in r_h and r_m determines the actual reaction rate. By comparing the values of corresponding parameters, we can get an idea about how variables in the discussion affect the reaction rate of the process too, obviously the same conclusion as that of numerical simulation holds. Moreover, even the extent to which the actual reaction rate depends on these variables is roughly consistent with the results of the simulation, that is $\delta > P_{in} \approx T_\infty > R_{in}$. Therefore, the two parameters newly introduced may describe the dynamic process in MH reactor quantitatively.

The configuration of a reactor affects the heat and mass transfer characteristics of the process, thus affects the actual reaction rate. Here TR, DR and ADR were chosen for discussion. First metal hydride in powders was supposed to be packed in the reactors, and the simulation results were shown in Fig. 9. In view of the performance the order of TR > DR > ADR was recognized, but the differences among them were not significant. Next the metal hydride in powders was replaced by compacts in order to enhance the heat transfer in the reactors, and the corresponding results were shown in Fig. 10. The order of TR > DR > ADR still held, but performances of the former two were obviously improved by packing compacts in the reactors while the opposite effect was observed for ADR, the gap in the performance between ADR and the other two reactors was thus widened. Why would the performance of ADR get even worse when packed with compacts? If we confine our discussion to the restriction of transport process on actual reaction rate, we may roughly conclude that mass transfer should be responsible for the result because heat transfer was undoubtedly improved by packing compacts in the reactor.

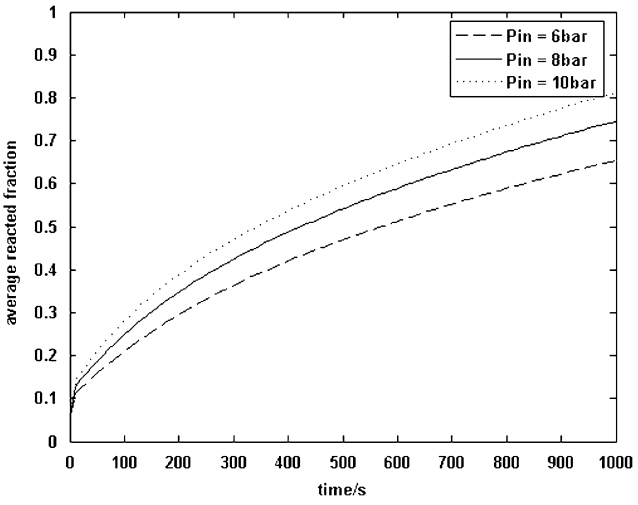

Fig. 7 – Performances for a TR under different inlet pressures.

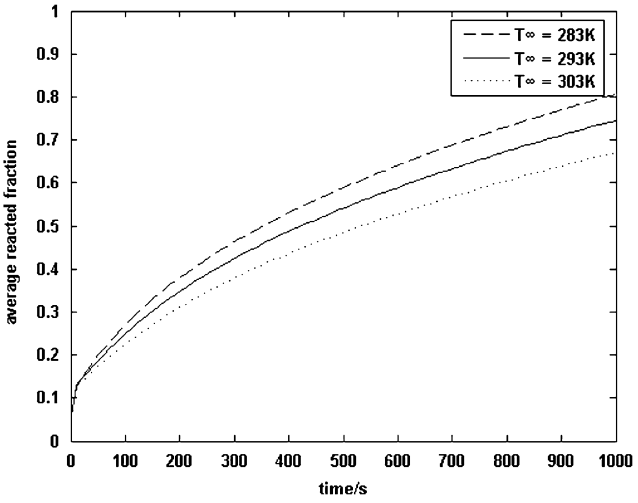

Fig. 8 – Performances for a TR under different heat transfer medium temperatures.

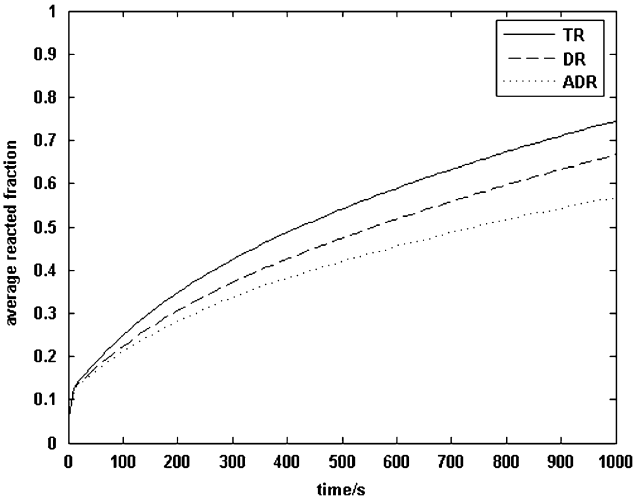

Fig. 9 – Performances for reactors of different configurations packed with powders.

Table 3 – The calculation results of r_h and r_m for TR with different design dimensions and operation conditions

	R_{in} (mm)			δ (mm)			P_{in} (bar)			T_∞ (K)		
	10	20	30	10	20	30	6	8	10	283	293	303
r_h, mol H_2/m^3 s	6.395	5.684	5.329	20.463	5.684	2.707	4.501	5.684	6.662	7.061	5.684	4.308
r_m, mol H_2/m^3 s	33 938	45 251	50 908	21 7206	45 251	17 238	23 115	45 251	74 603	49 674	45 251	38 947

In much the same way as discussions about the design dimensions and operation conditions, the effect of reactor configuration on the performance was studied by parameter analysis. Corresponding calculation results were listed in Table 4. The order in performance, namely TR > DR > ADR can be gained from the parameter comparison, too. Also, something else was revealed in the parameter analysis:

(1) For all the reactors packed with powders $r_h < r_m$ holds, thus heat transfer is the controlling step which mainly determines the actual reaction rate. However, the value of r_m for ADR is almost of the same order as the reaction rate calculated by essential kinetics, so its effect is not negligible. This is the reason why performance of the ADR is slightly lower than that of the DR.
(2) For reactors packed with compacts, different results arise. For TR and DR $r_h < r_m$ still holds while r_h is obviously increased, so the restriction of the transport process on actual reaction is loosened and the performances are improved correspondingly. For ADR packed with compacts, r_m is smaller than r_h, in other words, mass transfer becomes the controlling step of the actual reaction process under such situation, which coincides well with our former deduction in the numerical simulation. Moreover, the smaller one in r_h and r_m gets lower when powders in the reactor are replaced by compacts, therefore the transport process exerts more stringent restriction on actual reaction and the performance degrades.

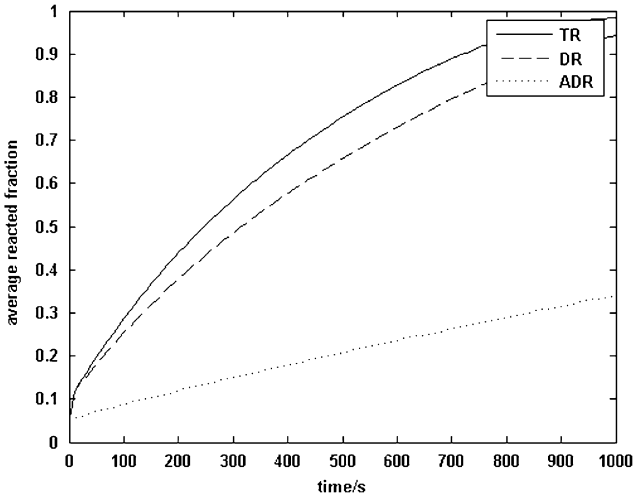

Fig. 10 – Performances for reactors of different configurations packed with compacts.

The usability of the two parameters introduced in the paper was demonstrated. They could catch the heat and mass transfer characteristics of MH reactor in a concise way. However, it should be noted that the method of parameter analysis is an approximation, and it will never take the place of numerical simulation for more detailed description of the process in MH reactor. In addition, some procedures of the formulation still need to be improved in accuracy in the future study.

5. Conclusions

Two parameters—heat transfer controlled reaction rate r_h and mass transfer controlled reaction rate r_m were proposed in the paper to describe the dynamic characteristics of the process in MH reactor. Then 2-D mathematical model of adsorption process was formulated and solved numerically. It was found by both numerical simulation and parameter analysis that smaller bed thickness, larger inlet pressure, lower temperature for heat transfer media favored the performance of MH reactor. The controlling step of process under given conditions was also discussed. Through comparison it is seen that the two parameters can be used to show the effects of many factors on the performance of MH reactor. Therefore, the introduction of the parameters provides a concise method for the performance analysis and the optimization of a MH reactor, thus may advance the application of various MH systems to a certain extent.

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Table 4 – The calculation results of r_h and r_m for TR, DR and ADR packed with powders and compacts, respectively

	Reactors packed with powders			Reactors packed with compacts		
	TR	DR	ADR	TR	DR	ADR
r_h, mol H_2/m^3 s	5.684	4.263	4.263	25.624	19.218	19.218
r_m, mol H_2/m^3 s	45 251	67 876	377.9	407.67	611.49	3.405

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