

Electromagnetic–thermal–mass transport triple hybrid model for energy-efficient hydrogen release from metal particles by induction heating

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Abstract

Hydrogen storage in metals is anticipated to be a highly promising technical approach for managing hydrogen in diverse energy applications, emphasizing the need to establish efficient operating conditions. In this study, we developed a numerical model that can simultaneously calculate hydrogen and heat transport combined with electromagnetic induction heating of metal particles. Using the developed numerical simulator, we investigated the behavior of the hydrogen release process from the hydrogen-absorbing metal and proposed important indicators for the operation. The fractions of the electromagnetic energy absorbed by the metal particle used for the hydrogen release, sensible heat, interfacial heat conduction, and thermal radiation were systematically evaluated. Considering the trade-off between temperature rise and the hydrogen concentration gradient, an optimal diameter of metal particles existed for the maximum hydrogen release rate. Similarly, the trade-off between temperature rise and energy consumption revealed an optimal electromagnetic power density for the heat utilization fraction for hydrogen release. Our electromagnetic–thermal–mass transport triple hybrid model constitutes a useful numerical simulator for the design of energy-efficient hydrogen storage systems.

Keywords

Hydrogen storage; Electrodynamics; Heat transfer; Modeling; Metal particle; Microwave;
Induction heating

1. Introduction

Hydrogen energy is positioned as an immensely significant fuel source for the future. However, there are substantial hurdles to its commercial realization at present, necessitating advancements in technology for hydrogen production, transportation, storage, and utilization. In terms of hydrogen production, various methods exist, including thermochemical, electrochemical, biological, and photocatalytic approaches [1–7]. Moreover, the combination of production methods and sources is identified through a color code [8–10]. Among these, the demand for environmentally friendly hydrogen production, known as 'green hydrogen', is expected to rise, emphasizing the importance of reducing the production cost of hydrogen derived from renewable energy sources like wind and solar power. Regarding hydrogen storage, it is categorized into gaseous, liquid, and solid forms, with solid hydrogen storage employing options such as metal hydrides, organometallic frameworks, and nanomaterials [3].

Hydrogen storage in metals is highly anticipated as a method of storing hydrogen, primarily due to their exceptional volumetric efficiency [11–15]. Furthermore, hydrogen storage in metals offers the advantage of safety, as it can be operated under relatively mild conditions, eliminating the risks of explosion associated with high-pressure hydrogen gas [12,15]. However, the drawbacks of hydrogen storage in metals include high material costs and low weight efficiency [12,14–16]. Hence, there is a pressing need to explore alloy systems with enhanced hydrogen storage capabilities and to establish more efficient operational methods.

In this study, we directed our attention to the hydrogen release process in Ti, a metal known for its exceptional volumetric efficiency in hydrogen storage [17–19]. Previously, we had developed a numerical model for hydrogen transport in Ti consisting of surface

adsorption, subsurface transport, and bulk diffusion kinetics [20]. However, this model was limited to constant temperature conditions and did not account for external heating and the associated heat transport. Therefore, in the present study, we undertook kinetic modeling of the electromagnetic induction heating of Ti particles and the associated hydrogen release process. For hydrogen storage in metals, while the absorption of hydrogen can occur at relatively low temperatures, the release process usually demands elevated temperatures to sufficiently shift the thermal equilibrium and ensure a practical release rate. This necessity poses a significant bottleneck in solid-state hydrogen storage. Consequently, there is a critical need to explore more efficient hydrogen release strategies. Electromagnetic induction heating, a method utilizing the application of a magnetic field, allows for the selective heating of targeted Ti particles that absorb hydrogen [21,22]. Thereby this induction heating scheme can achieve high energy efficiency and minimize the equipment degradation in the hydrogen release process. In particular, we aimed to develop a triple hybrid model that comprehensively and numerically analyzes multiple interrelated physical phenomena: energy absorption by metal particles from electromagnetic fields, heat transport around particles, and hydrogen transport, which is intricately coupled with these processes and highly temperature-dependent.

The model developed in this study also holds potential for applications in nuclear fusion energy generating systems. As a candidate for a blanket, which is one of the components of a fusion reactor, a system in which molten salt containing Ti particles are circulated was proposed [21–26]. In this system, the Ti particles absorb tritium generated from the reaction between neutrons released from the core and lithium nuclei in the molten salt. Subsequent heating causes the Ti particles to release tritium, enabling the reuse of scarce tritium as the fusion reaction fuel. In a molten salt environment with low tritium solubility, Ti particles serve as effective tritium transport media, contributing to increased tritium solubility in the

blanket and enhanced safety by preventing tritium permeation outside the blanket. Moreover, this system makes it possible to employ low activation vanadium alloys, which possess high mechanical strength but tend to absorb tritium, as structural materials for the blanket. In operating a molten salt blanket containing Ti particles, developing a technology to release the tritium absorbed by the Ti particles is indispensable. In this context, electromagnetic induction heating can be a promising scheme for the extraction of tritium from the Ti particles.

In the present study, we develop a numerical model that can simultaneously calculate hydrogen and heat transport combined with electromagnetic induction heating of metal particles. To the best of our knowledge, this is the first numerical model of hydrogen transport that handles the electromagnetic energy transfer, heat transfer, and mass transfer. Our electromagnetic–thermal–mass transport triple hybrid model may provide a useful numerical simulator for the design of metal-based hydrogen storage systems with accelerated and energy-efficient hydrogen release by using electromagnetic induction heating.

2. Theory and calculation methods

Table 1 lists the symbols used in the formulation of this study. The fundamental concept of the numerical model of hydrogen transport in flat Ti is described in Ref. 20, and its extension to spherical Ti is depicted schematically in Fig. 1. The hydrogen mass balances are formulated as

$$X_{max} N_s \frac{d\theta}{dt} = J_{ads} - J_{des} - J_{sb} + J_{bs}, \quad (1)$$

$$X_{max} N_s \frac{d\theta_{ss}}{dt} = J_{sb} - J_{bs} - J_{dif} \Big|_{subsurface}, \quad (2)$$

$$\frac{N_b V}{A} \frac{dX}{dt} = J_{sb} - J_{bs}. \quad (3)$$

The upper limit of hydrogen molar fraction in Ti, denoted as X_{max} [mol-H/mol-Ti], was established at 3 in this study [20,27–29]. To provide further insight, it is essential to consider the β phase of Ti, characterized by a body-centered cubic structure containing two Ti atoms per unit cell. Within this structure, there are 24 tetrahedral sites on the unit cell's surface, allowing for a maximum of 12 atoms to occupy these sites. However, due to the site-blocking effect, hydrogen atoms can occupy only half of the tetrahedral sites. Consequently, the highest possible number of hydrogen atoms within a unit cell is six, resulting in $X_{max} = 3$. It is noteworthy that for the α and δ phases, the corresponding values are 1 and 2, respectively. A more detailed explanation can be found in Ref. 20. N_s is the molar density of Ti per surface area. θ is the fractional coverage, or occupancy, of hydrogen atoms at the surface. J_{ads} and J_{des} are the hydrogen fluxes for the surface adsorption and desorption processes, respectively. J_{sb} and J_{bs} are the hydrogen fluxes for the inward and outward subsurface transport, respectively. θ_{ss} is the fractional coverage of hydrogen atoms at the subsurface. J_{dif} is the hydrogen flux for the diffusion in the bulk region. N_b is the molar density of Ti per volume. V and A are the volume and surface area of Ti, respectively. X [mol-H/mol-Ti] is the hydrogen molar fraction in Ti. The values of N_s and N_b are calculated by

$$N_s = \frac{(N_A N_b)^{\frac{2}{3}}}{N_A}, \quad (4)$$

$$N_b = \frac{\rho}{M}, \quad (5)$$

where N_A is the Avogadro constant, ρ is the mass density of Ti, and M is the molar mass of Ti. Consequently, N_s and N_b are equal to $2.45 \times 10^{-5} \text{ mol m}^{-2}$ and $9.4 \times 10^4 \text{ mol m}^{-3}$, respectively. The values of J_{dif} , J_{bs} , J_{sb} [30], J_{des} , and J_{ads} [31] are determined by

$$J_{dif} = D_H^0 \frac{\partial C(r, t)}{\partial r} \exp\left(-\frac{E_{dif}}{RT_s}\right), \quad (6)$$

$$J_{bs} = k_{bs}^0 X_{max} N_s \theta_{ss} (1 - \theta) \exp\left(-\frac{E_{bs}}{RT_s}\right), \quad (7)$$

$$J_{sb} = k_{sb}^0 X_{max} N_s \theta (1 - \theta_{ss}) \exp\left(-\frac{E_{sb}}{RT_s}\right), \quad (8)$$

$$J_{des} = k_{des}^0 \theta^2 \exp\left(-\frac{E_{des}}{RT_s}\right), \quad (9)$$

$$J_{ads} = 2S_0 (1 - \theta)^2 \frac{P_{H_2}}{\sqrt{2\pi M_{H_2} RT_g}}. \quad (10)$$

D_H^0 ($9.0 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ [32]) is the prefactor of the diffusion coefficient of hydrogen. $C(r, t)$ is the local concentration of hydrogen in the bulk. r represents the center-based coordinates of a spherical Ti particle, and $C(r, t)$ is calculated for each parcel delimited by a specified

number of meshes between the center of the sphere and the surface. E_{dif} (5.2×10^4 J mol⁻¹ [32]), E_{bs} (8.5×10^4 J mol⁻¹ [20]), E_{sb} (1.2×10^5 J mol⁻¹ [20]), and E_{des} (1.17×10^5 J mol⁻¹ [31]) are the activation energy values of hydrogen for diffusion in the bulk region, the outward and inward subsurface transport, and the surface desorption, respectively. k_{bs}^0 (3.24×10^9 s⁻¹ [20]), k_{sb}^0 (1.16×10^{11} s⁻¹ [20]), and k_{des}^0 (1.08×10^8 mol m⁻² s⁻¹ [31]) are the frequency factors for the outward and inward subsurface transport of hydrogen atoms, and the surface desorption, respectively. T_s and T_g are the absolute temperatures of the solid and gas phase, respectively. S_0 is the sticking coefficient at zero coverage of hydrogen atoms onto the surface of Ti. P_{H_2} and M_{H_2} are the partial pressure and molar mass of hydrogen, respectively. R is the ideal gas constant. S_0 is unitless for Eq. (10) in the SI unit system and given by

$$S_0 = 0.0143 \exp\left(-\frac{E_{S_0}}{RT_s}\right), \quad (11)$$

where E_{S_0} (-1.99×10^3 J mol⁻¹ [31,33]) is the (regressive) activation energy value for the initial chemisorption [31,33]. In our previous study, experimental data of hydrogen absorption into flat Ti in Ref. 34 were numerically simulated based on the hydrogen transport model [20]. The experimental data for the hydrogen absorption process in Ti at several temperatures could be reproduced with a single set of kinetic parameters. Furthermore, using the determined kinetic parameters allowed us to reproduce the experimental data also for the hydrogen desorption process from Ti at multiple temperatures in Ref. 34, confirming the validity of the hydrogen transport model [20].

Table. 1. List of the symbols, their definitions, and units used in the formulation.

A	Surface area of Ti	[m ²]
B_0	Amplitude of magnetic flux density	[T]
C	Local concentration of hydrogen in the bulk	[mol-H m ⁻³]
C_p	Specific heat capacity of Ti	[J kg ⁻¹ K ⁻¹]
d	Diameter of Ti particle	[m]
D_H^0	Prefactor of diffusion coefficient of hydrogen	[m ² s ⁻¹]
E_{bs}	Activation energy for outward subsurface transport of hydrogen	[J/mol-H]
E_{des}	Activation energy for surface desorption of hydrogen	[J/mol-H]
E_{dif}	Activation energy for diffusion of hydrogen in the bulk region	[J/mol-H]
E_{sb}	Activation energy for inward subsurface transport of hydrogen	[J/mol-H]
E_{S0}	Activation energy for initial chemisorption	[J/mol-H]
h	Heat transfer coefficient between Ti particles and gas phase	[W m ⁻² K ⁻¹]
J_{ads}	Hydrogen flux for surface adsorption	[mol-H m ⁻² s ⁻¹]
J_{bs}	Hydrogen flux for outward subsurface transport	[mol-H m ⁻² s ⁻¹]
J_{des}	Hydrogen flux for surface desorption	[mol-H m ⁻² s ⁻¹]
J_{dif}	Hydrogen flux for diffusion in bulk region	[mol-H m ⁻² s ⁻¹]
J_{sb}	Hydrogen flux for inward subsurface transport	[mol-H m ⁻² s ⁻¹]
k	Thermal conductivity of hydrogen gas	[W m ⁻¹ K ⁻¹]
k_0	Thermal conductivity of hydrogen gas at standard atmospheric pressure	[W m ⁻¹ K ⁻¹]
k_{bs}^0	Frequency factor for outward subsurface transport of hydrogen atoms	[s ⁻¹]
k_{des}^0	Frequency factor for surface desorption of hydrogen atoms	[mol-H m ⁻² s ⁻¹]
k_{sb}^0	Frequency factor for inward subsurface transport of hydrogen atoms	[s ⁻¹]
M	Molar mass of Ti	[kg mol ⁻¹]
M_{H2}	Molar mass of hydrogen	[kg/mol-H ₂]
N_A	Avogadro constant	[mol ⁻¹]
N_b	Molar density of Ti per volume	[mol m ⁻³]
N_s	Molar density of Ti per surface area	[mol m ⁻²]
Nu	Nusselt number	[–]
P_{H2}	Partial pressure of hydrogen	[Pa]
P_0	Standard atmospheric pressure	[Pa]
r	Center-based coordinates of a spherical Ti particle	[m]
R	Ideal gas constant	[J mol ⁻¹ K ⁻¹]
S_0	Sticking coefficient of hydrogen atoms onto Ti surface	[–]
t	Time	[s]
T_g	Absolute temperature of gas phase	[K]
T_s	Absolute temperature of solid phase	[K]
T_{S0}	Initial absolute temperature of solid phase	[K]
v	Hydrogen release rate	[mol m ⁻³ s ⁻¹]
v_{ave}	Average hydrogen release rate	[mol m ⁻³ s ⁻¹]
V	Volume of Ti	[m ³]

W_H	Power consumption of electromagnetic induction heating	[W]
X	Hydrogen molar fraction in Ti	[-] (mol-H/mol-Ti)
X_{max}	Maximum hydrogen molar fraction in Ti	[-] (mol-H/mol-Ti)
X_0	Initial hydrogen molar fraction in Ti	[-] (mol-H/mol-Ti)
δ	Skin depth of Ti particle	[m]
ΔH_{abs}	Absorption enthalpy of hydrogen into Ti	[J/mol-H]
ε	Emissivity of Ti	[-]
η_{cond}	Heat utilization fraction for interfacial heat conduction	[-]
η_{hyd}	Heat utilization fraction for hydrogen release	[-]
η_{rad}	Heat utilization fraction for thermal radiation	[-]
η_{sen}	Heat utilization fraction for sensible heat	[-]
θ	Fractional coverage of hydrogen atoms at Ti surface	[-]
θ_{ss}	Fractional coverage of hydrogen atoms at the subsurface	[-]
μ_m	Permeability of hydrogen gas	[H m ⁻¹]
μ_0	Permeability of vacuum	[H m ⁻¹]
ν	Frequency of the field	[s ⁻¹]
ρ	Mass density of Ti	[kg m ⁻³]
σ	Electrical conductivity of Ti	[Ω^{-1} m ⁻¹]
σ_{SB}	Stefan–Boltzmann constant	[W m ⁻² K ⁻⁴]

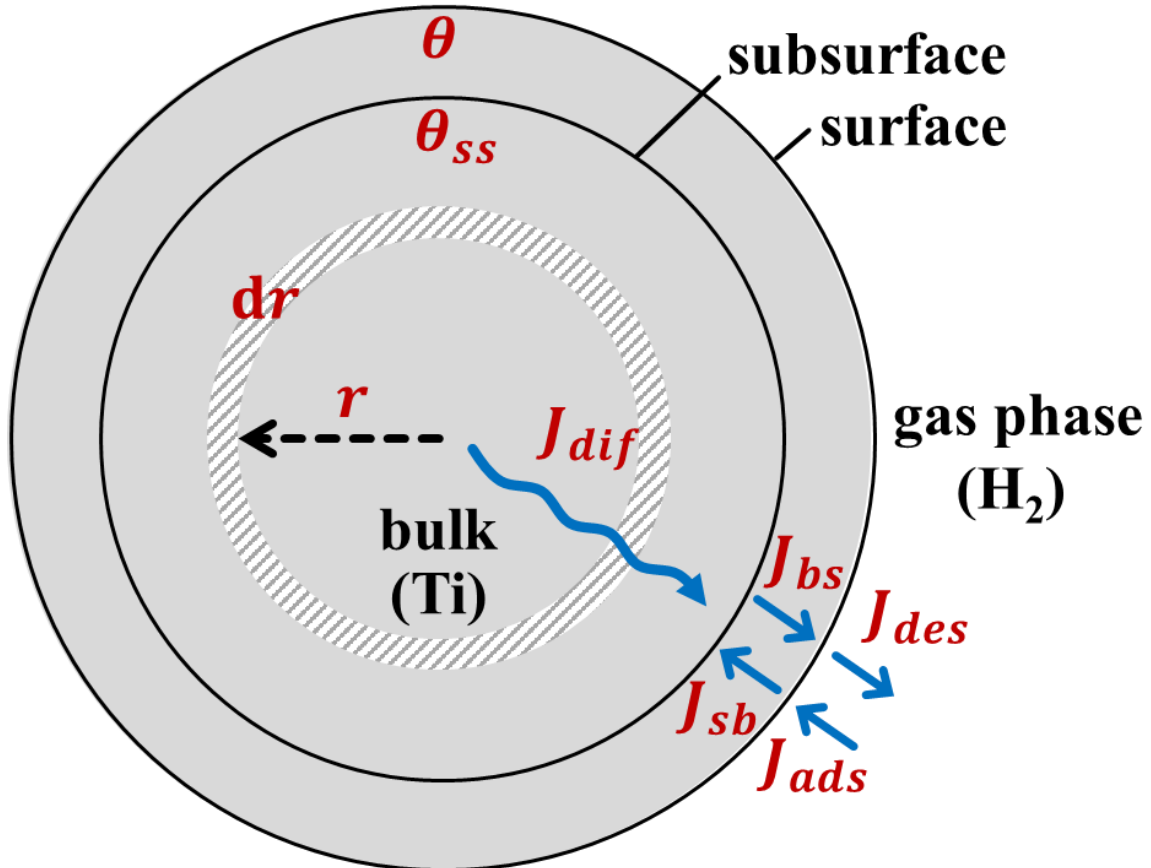


Fig. 1. Conceptual schematic diagram of our calculation model for hydrogen absorption into Ti. J_{dif} is the hydrogen flux for diffusion in the bulk region; J_{bs} and J_{sb} are the fluxes for the migration of hydrogen from the subsurface to the surface, and from the surface to the subsurface, respectively; J_{des} and J_{ads} are the hydrogen fluxes for the surface adsorption and desorption processes, respectively; θ and θ_{ss} are the fractional coverage at the surface and subsurface, respectively; and r is the distance from the center of the spherical Ti particle.

Due to the considerably lower thermal conductivity of hydrogen gas compared to that of Ti particles, heat transfer within the Ti particles is predominantly governed by the interface between the atmospheric hydrogen gas and the Ti particles. Consequently, internal heat conduction within the Ti particles is considered negligible, and the temperature distribution within the Ti particles is assumed to be uniform. The heat balance of Ti is formulated as

$$C_p \rho V \frac{dT_s}{dt} = W_H - \Delta H_{abs} (J_{sb} - J_{bs}) A - h(T_s - T_g) A - \varepsilon \sigma_{SB} T_s^4 A. \quad (12)$$

C_p ($5.22 \times 10^2 \text{ J kg}^{-1} \text{ K}^{-1}$) is the specific heat capacity of Ti. W_H is the power consumption of electromagnetic induction heating. ΔH_{abs} ($-6.26 \times 10^4 \text{ J mol}^{-1}$ [35]) is the absorption enthalpy of hydrogen into Ti. h is the heat transfer coefficient between the Ti particles and the gas phase. ε (0.63) is the emissivity of Ti. σ_{SB} is the Stefan–Boltzmann constant. Concerning the right-hand side of Eq. (12), the first term represents the electromagnetic induction heating contribution, the second term represents the endothermic effect associated with hydrogen release from Ti, the third term represents the interfacial heat conduction between Ti particles and hydrogen gas, and the fourth term represents the thermal radiation contribution. Electromagnetic induction heating refers to Joule heating within a metal induced

by an inductive electric field generated by an externally applied magnetic field. This technique enables the selective heating of only the desired Ti particles responsible for hydrogen absorption. This approach not only achieves high energy efficiency but also reduces equipment degradation by avoiding the exposure of the components other than the Ti particles to the elevated temperatures required for hydrogen release. In this study, we utilized an AC magnetic field with a wavelength significantly larger than the particle size, assuming that the Ti particle is positioned at an antinode of the standing wave of magnetic field. The power absorbed by the spherical particle in this scenario is described by the following equation [23]:

$$W_H = \frac{36\pi B_0^2 \nu V}{\mu_m} \left(\frac{\delta}{d} \right)^2 \left[\frac{d}{2\delta} \frac{\sinh(d/\delta) + \sin(d/\delta)}{\cosh(d/\delta) - \cos(d/\delta)} - 1 \right]. \quad (13)$$

B_0 is the amplitude of magnetic flux density. ν is the frequency of the field. μ_m ($1.26 \times 10^{-6} \text{ H m}^{-1}$) is the permeability of the hydrogen gas. d is the diameter of the Ti particle. δ is the skin depth of the Ti particle ($\delta = 1/\sqrt{\pi\mu_0\sigma\nu}$; μ_0 is the permeability of vacuum, and σ ($7.14 \times 10^5 \text{ } \Omega^{-1} \text{ m}^{-1}$ [36,37]) is the electrical conductivity of Ti) [23,38–40]. To determine h between the Ti particles and hydrogen gas, we account for the Nusselt number Nu ($= hd/k$; k is the thermal conductivity of hydrogen gas). Then, we can determine h by $h = kNu/d$. It is theoretically known that $Nu = 2$ in stationary systems where the relative velocity between the spherical particle and the surrounding medium is small, or they move together [23,41]. Therefore, in the present study, h is determined by

$$h = \frac{2k}{d}. \quad (14)$$

As the pressure dependence of k , we simply assume

$$k = k_0 \frac{P_{H_2}}{P_0}, \quad (15)$$

where k_0 ($0.18 \text{ W m}^{-1} \text{ K}^{-1}$) is the thermal conductivity of hydrogen gas at standard atmospheric pressure, and P_0 (1 atm) is the standard atmospheric pressure.

In the numerical simulations, the hydrogen fluxes at each time step, obtained by Eqs. (6)–(10), are employed to calculate $\theta, \theta_{ss}, X, C(r, t)$, and T_s at the next time step by solving each balance equation using the fourth-order Runge–Kutta method. The shape of Ti particle is assumed to be a sphere with a finite radius, and hydrogen transport is considered solely in the radial direction from the center of the sphere due to the point symmetry. Here, the number of meshes between the center and the surface of the Ti particle is set to 100, with a mesh size of $dr = (d/2)/100 = d/200$. At $r = 0$, we have the center of the Ti particle, and at $r = dr \times 100 = d/2$, we encounter the mesh nearest to the surface, defining the subsurface region. In this subsurface region, the hydrogen concentration is proportional to θ_{ss} , and is calculated as

$$C\left(\frac{d}{2}, t\right) = \theta_{ss} X_{max} N_b. \quad (16)$$

3. Results and discussion

The typical behavior of spherical Ti particle with stored hydrogen when subjected to electromagnetic induction heating was simulated based on the constructed numerical model.

The simulation conditions assumed a constant hydrogen gas atmosphere at $P_{H_2} = 0.1$ atm and $T_g = 25^\circ\text{C}$. Ti particles with $d = 3$ mm with initial conditions $T_{s0} = 25^\circ\text{C}$ and $X_0 = 1.5$ were exposed to a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$. Here, T_{s0} and X_0 represent the initial Ti temperature and the initial hydrogen molar fraction in Ti, respectively. The initial hydrogen concentration distribution within the Ti particles was assumed to be uniform, given by $C(r, 0) = X_0 N_b$. For electromagnetic induction heating, it is known that $W_H/(B_0^2 \nu V)$ reaches its maximum when $d/\delta = 4.818$ from Eq. (13) [23]. In this study, ν was set to satisfy this condition (n.b., δ is dependent on ν , as described above.), with B_0 configured such that $B_0^2 \nu = 100 \text{ T}^2 \text{ s}^{-1}$.

Fig. 2 shows the time evolution of X and T_s . Following the onset of heating, the increase of T_s is primarily driven by the contributions of the first, third, and fourth terms on the right-hand side of Eq. (12), with little influence on the hydrogen absorption enthalpy. As T_s reaches a certain level, the hydrogen release rate increases, leading to a reduction of X . At this point, the contribution of the second term on the right-hand side of Eq. (12), the effect of absorption enthalpy, becomes sufficiently large, and the increase of T_s continues based on the contributions of all terms on the right-hand side of Eq. (12). As X approaches equilibrium, the hydrogen release rate becomes small and X remains constant. At this time, T_s is constant at a level where the sum of the first, third, and fourth terms on the right-hand side of Eq. (12) is zero. This equilibrium signifies a balance between energy absorption from the electromagnetic field to the Ti particles due to the electromagnetic induction heating and the energy release from the Ti particles due to heat transfer through the Ti surfaces. Fig. 3 illustrates the time evolution of $C(r)$. Since hydrogen is only released from the Ti particle surfaces, $C(r)$ near the Ti particle surfaces decreases as T_s increases. Hydrogen release always proceeds with a hydrogen concentration gradient, and when the hydrogen

concentration gradient disappears, hydrogen release halts, leading to an equilibrium state.

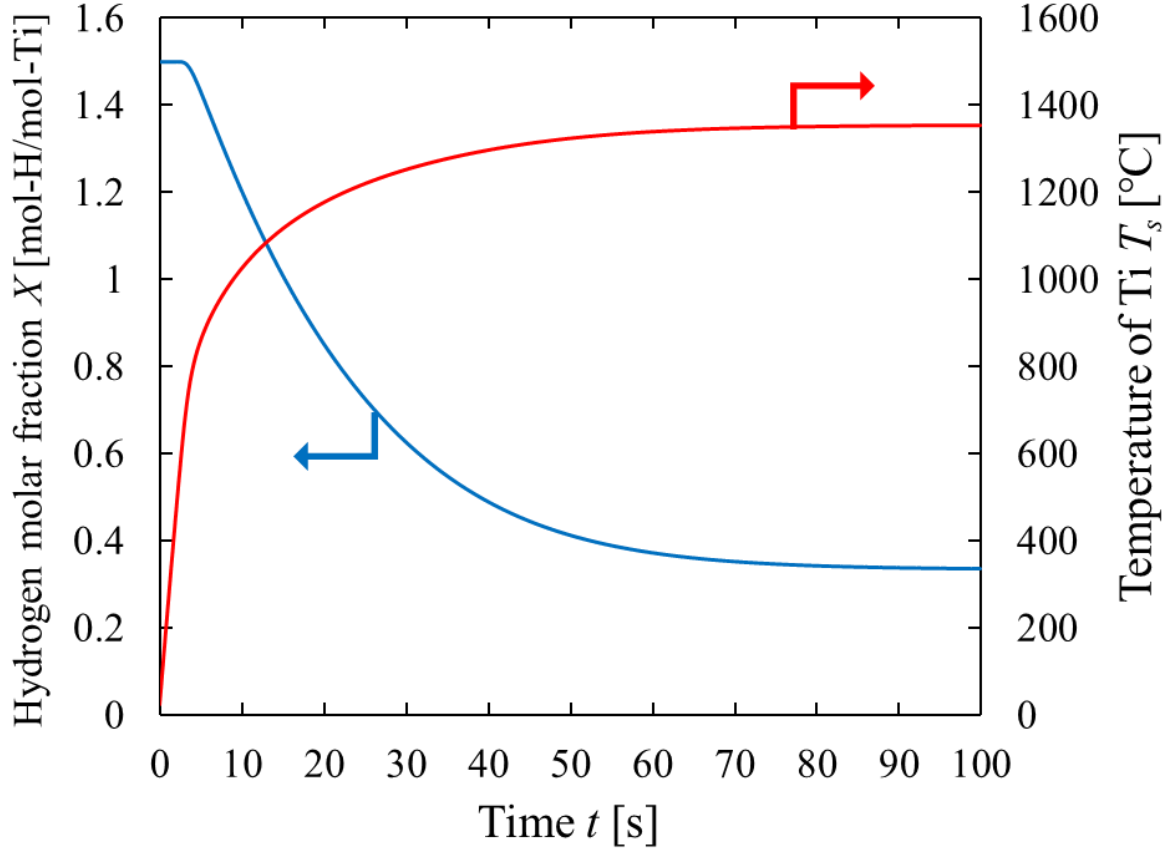


Fig. 2. Time evolution of X and T_s in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

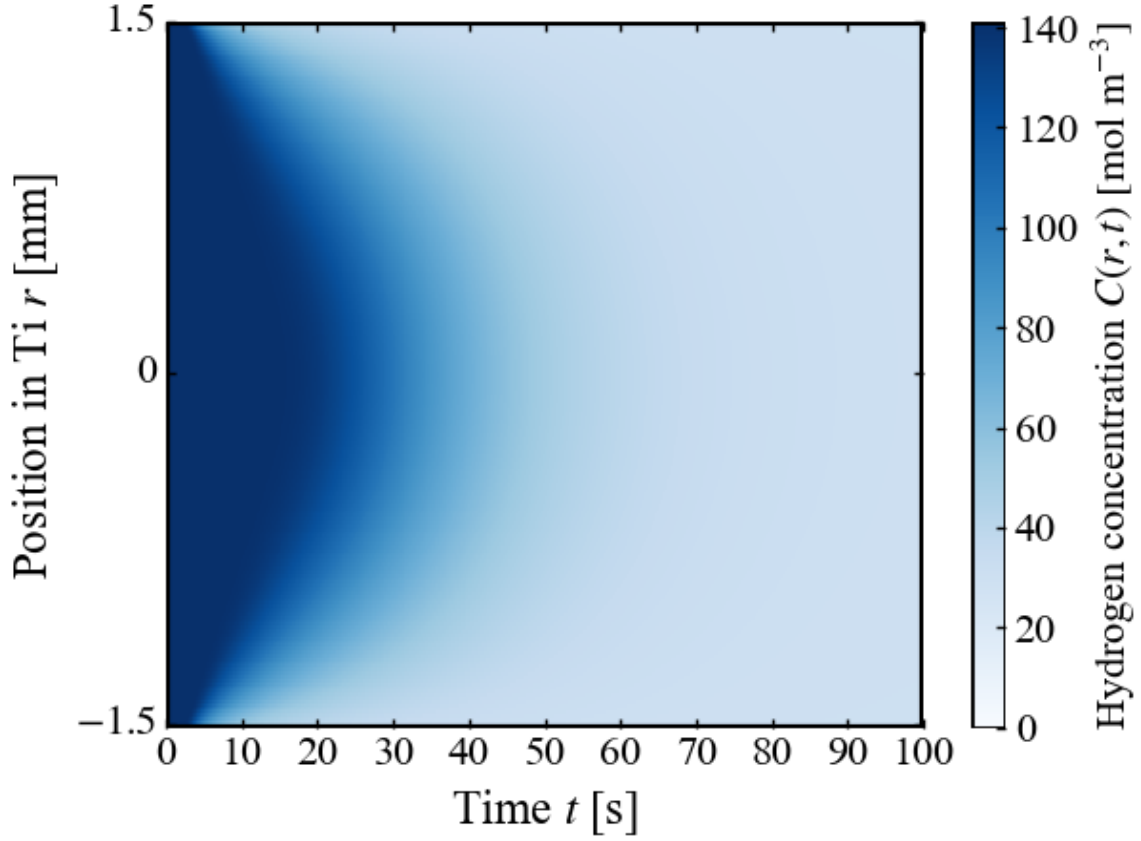


Fig. 3. Time evolution of $C(r)$ in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

Fig. 4 shows the time evolution of hydrogen release rate, denoted as ν , calculated as

$$\nu = -N_b \frac{dX}{dt} = \frac{(J_{bs} - J_{sb})A}{V}. \quad (17)$$

Immediately after the start of heating, ν is minimal due to the low T_s . Over time, as T_s increases and hydrogen motion becomes more active, ν rises. However, as hydrogen release progresses, it gradually approaches an equilibrium state, leading to a deceleration in the release rate. Due to such an evolving mechanism, following the initiation of heating, ν starts

from around zero, reaches a peak at a certain point in time, and then gradually decreases, ultimately converging towards zero. Here, we define the average hydrogen release rate, denoted as v_{ave} , calculated as

$$v_{ave} = \frac{\int_0^t v dt}{t}. \quad (18)$$

v_{ave} can also be expressed by the following equation:

$$v_{ave} = \frac{(X_0 - X) N_b}{t}. \quad (19)$$

Fig. 5 shows the calculated time evolution of v_{ave} for the given condition. The time at which v_{ave} reaches its maximum is later than the time when v is at its maximum. When considering the operational conditions of hydrogen storage in metals, v_{ave} is a more crucial indicator than v . From an energy perspective, it is efficient to continue heating at least until the time when v_{ave} reaches its maximum.

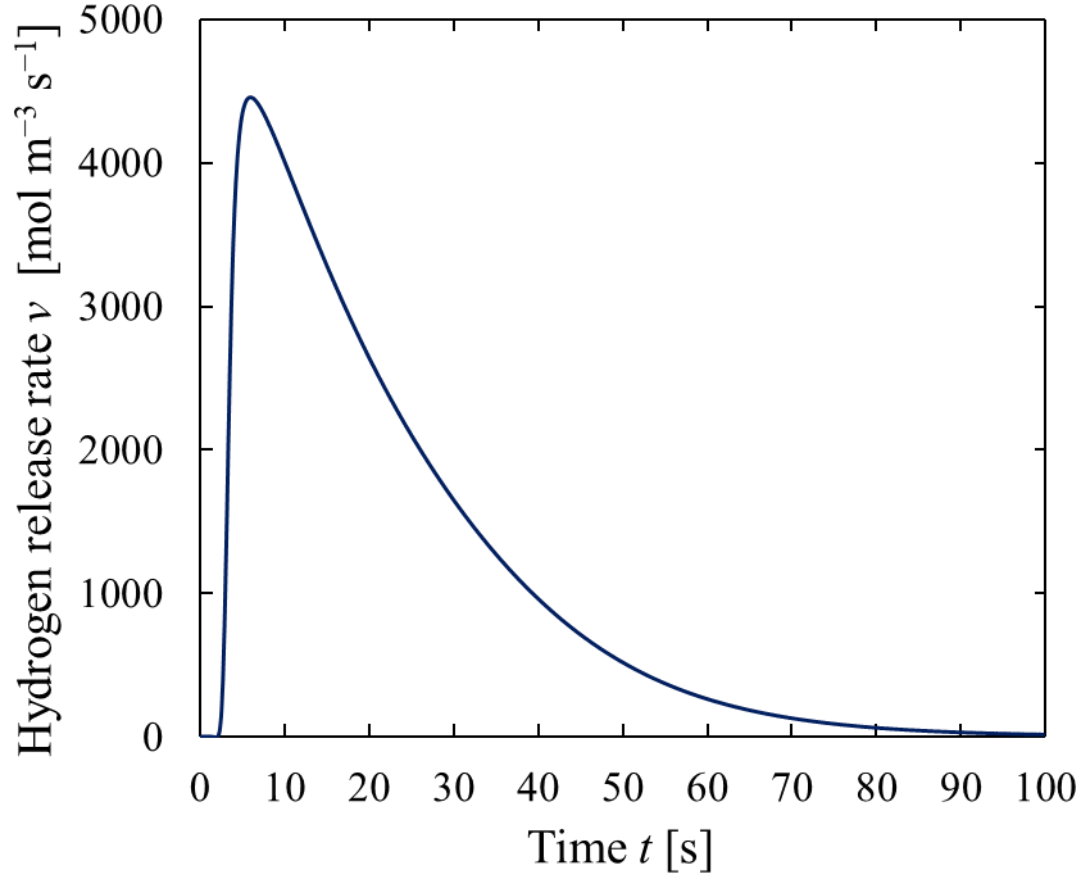


Fig. 4. Time evolution of v in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

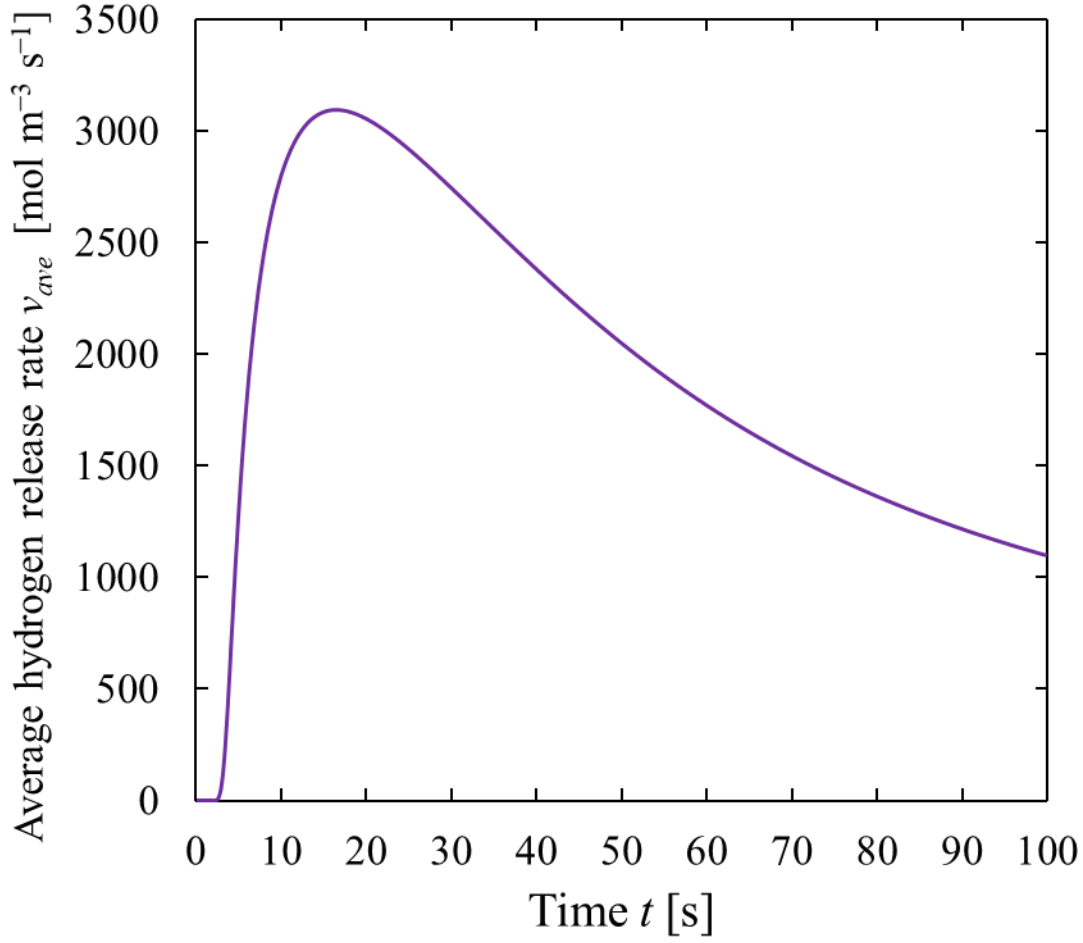


Fig. 5. Time evolution of v_{ave} in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

We also define the heat utilization fraction for hydrogen release, denoted as η_{hyd} , which is expressed as

$$\eta_{hyd} = -\frac{\Delta H_{abs} (X_0 - X) N_b V}{W_H t}. \quad (20)$$

This is an important factor for the energy efficiency evaluation that represents how much

energy is utilized for the release of hydrogen from the Ti particle out of the applied electromagnetic energy. From Eqs. (19) and (20), η_{hyd} is expressed by the following equation using v_{ave} :

$$\eta_{hyd} = -\frac{\Delta H_{abs} v_{ave} V}{W_H}. \quad (21)$$

Alternatively, η_{hyd} can be expressed through Eqs. (17), (18), and (21) as follows using the second term on the right-hand side of Eq. (12):

$$\eta_{hyd} = \frac{\int_0^t \Delta H_{abs} (J_{sb} - J_{bs}) A dt}{W_H t}. \quad (22)$$

Fig. 6 shows the calculated time evolution of η_{hyd} . Immediately after the start of heating, v is small due to the low T_s , and η_{hyd} is close to zero. As time passes, T_s rises and hydrogen release progresses, with η_{hyd} reaching its maximum when v_{ave} peaks as understood from Eq. (21). Hereafter, we denote this maximum η_{hyd} in time as $\eta_{hyd,max}$. As equilibrium is approached, η_{hyd} approaches zero as the total hydrogen release remains constant while the electromagnetic power consumption increases in proportion to the elapsed time. From an energy perspective, heating the Ti particles for hydrogen release until the time of maximum η_{hyd} can be considered ideal. Here, we further define the heat utilization fraction for sensible heat (η_{sen}), interfacial heat conduction (η_{cond}), and thermal radiation (η_{rad}) as

$$\eta_{sen} = \frac{C_p \rho V (T_s - T_{s0})}{W_H t}, \quad (23)$$

$$\eta_{cond} = \frac{\int_0^t h(T_s - T_g) A dt}{W_H t}, \quad (24)$$

$$\eta_{rad} = \frac{\int_0^t \epsilon \sigma_{SB} T_s^4 A dt}{W_H t}. \quad (25)$$

The sum of η_{hyd} , η_{sen} , η_{cond} , and η_{rad} is always 1 because the energy consumption of electromagnetic induction heating is used for one of the following: hydrogen release, sensible heat, interfacial heat conduction, and thermal radiation. Fig. 7 presents the calculated time evolution of η_{hyd} , η_{sen} , η_{cond} , and η_{rad} . Immediately after the initiation of heating, η_{hyd} , η_{cond} , and η_{rad} are small because of the low T_s , and most of the heat is utilized for the sensible heat required for the temperature increase of Ti particle. For our initial condition setting, T_s starts at 25°C, which is equal to T_g , and afterward T_s always increases, so η_{cond} and η_{rad} are also observed to consistently increase.

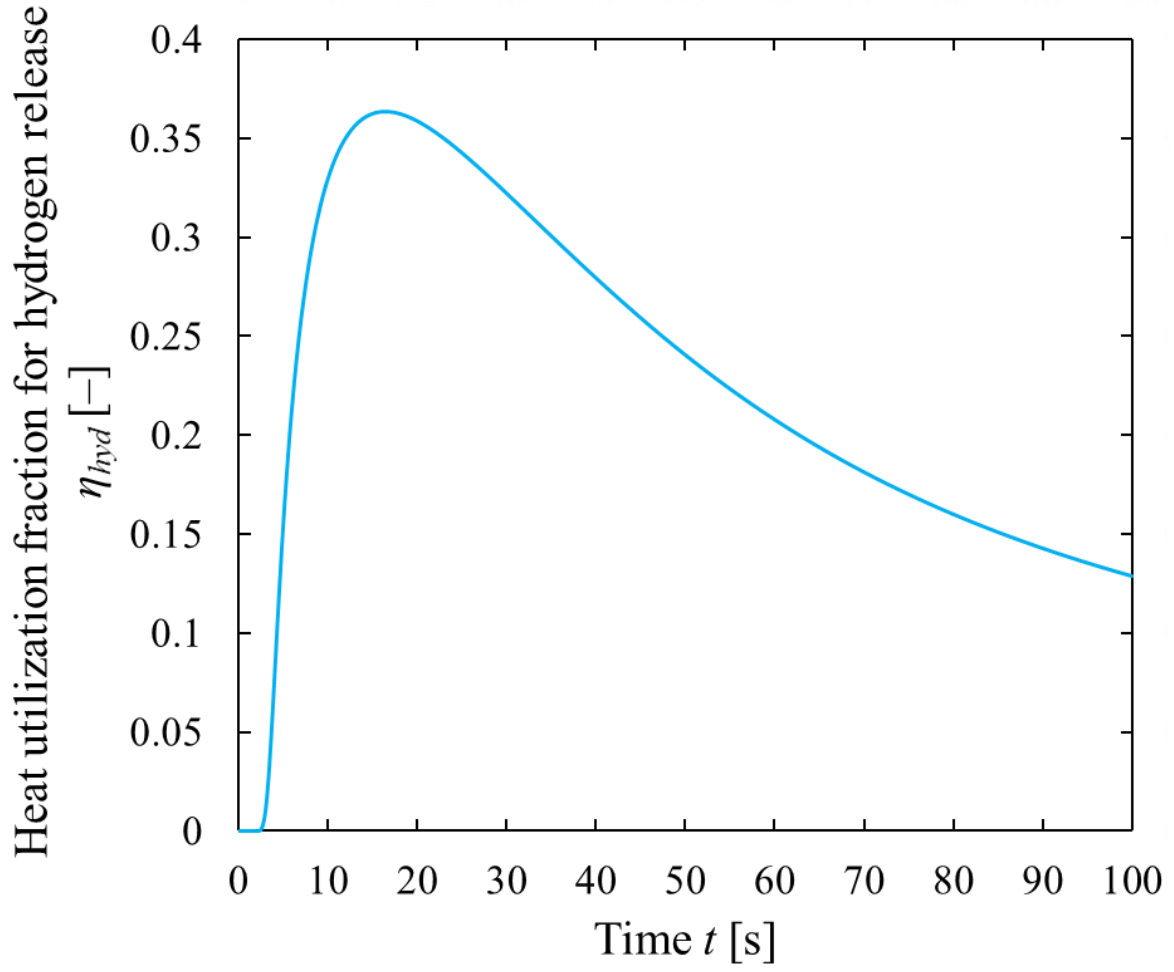


Fig. 6. Time evolution of η_{hyd} in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

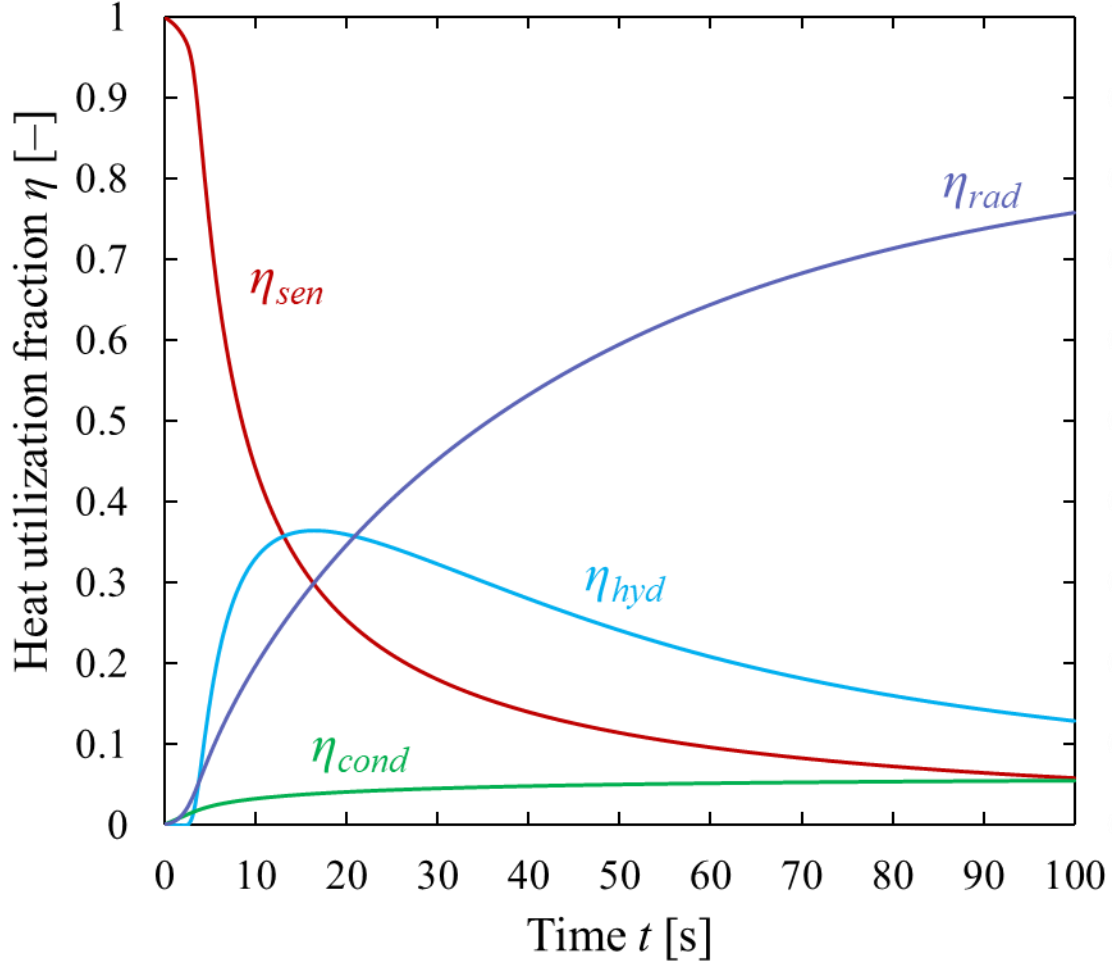


Fig. 7. Time evolution of η_{hyd} , η_{sen} , η_{cond} , and η_{rad} in a Ti particle with $d = 3$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $\nu = 9.15 \times 10^5 \text{ s}^{-1}$ and $B_0 = 1.05 \times 10^{-2} \text{ T}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

We searched for conditions that maximize η_{hyd} by changing d and W_H/V . In other words, we explored the optimization of η_{hyd} concerning three variables: diameter of Ti particle (d), power density (W_H/V), and heating time (t). The simulation conditions assumed a constant hydrogen gas atmosphere at $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$. Ti particles with different diameters with initial conditions $T_{s0} = 25^\circ\text{C}$ and $X_0 = 1.5$ were exposed to

magnetic fields of different power densities. The initial hydrogen concentration distribution within the Ti particles was assumed to be uniform, given by $C(r, 0) = X_0 N_b$. Fig. 8 presents $\eta_{hyd,max}$ for each condition of $d = 100, 150, 200, 250, 300 \mu\text{m}$ and $W_H/V = 50, 100, \dots, 450, 500 \text{ GW m}^{-3}$. In Eq. (12), the first term on the right-hand side, which is proportional to the volume of the particle, acts to heat the particle, and the second, third, and fourth terms, which are proportional to the surface area of the particle, act to cool the particle. Therefore, the larger d (i.e., the smaller the specific surface area), the more dominant the heating becomes, making it easier to release hydrogen in terms of temperature. However, the larger d , the smaller the hydrogen concentration gradient within the Ti particle, and thus the lower the hydrogen release rate becomes in terms of the driving force of diffusion. Due to such a trade-off in the influence of the particle diameter on the hydrogen release rate, η_{hyd} becomes its maximum at an intermediate d for each W_H/V , as observed in Fig. 8. The larger W_H/V , the easier it is to raise T_s and release hydrogen, but the more energy is required. Therefore η_{hyd} is maximum at an intermediate W_H/V for each d . This situation is closely related to the fact that there is a heating time at which η_{hyd} is maximum for each condition, as observed in Fig. 6. Under the given conditions, applying a magnetic field with $W_H/V = 150 \text{ GW m}^{-3}$ to Ti particles with $d = 150 \mu\text{m}$ results in $\eta_{hyd} = 0.512$ at $t = 7.61 \times 10^{-2} \text{ s}$. This represents the condition with the highest η_{hyd} among all combinations of d , W_H/V , and t . Fig. 9 shows the time evolution of T_s , X , and η_{hyd} when a magnetic field of $W_H/V = 150 \text{ GW m}^{-3}$ is applied to Ti particles with $d = 150 \mu\text{m}$, the condition that results in the maximum η_{hyd} . Initially, $T_s = 25^\circ\text{C}$ and $X_0 = 1.5$. Then, at $t = 7.61 \times 10^{-2} \text{ s}$, when η_{hyd} peaks, T_s rises to 1724°C , and X drops to 0.51. Although theoretically, inducing hydrogen release under these conditions is energetically optimal, such a rapid change in the material temperature may make it impractical as an operating condition due to safety and control considerations.

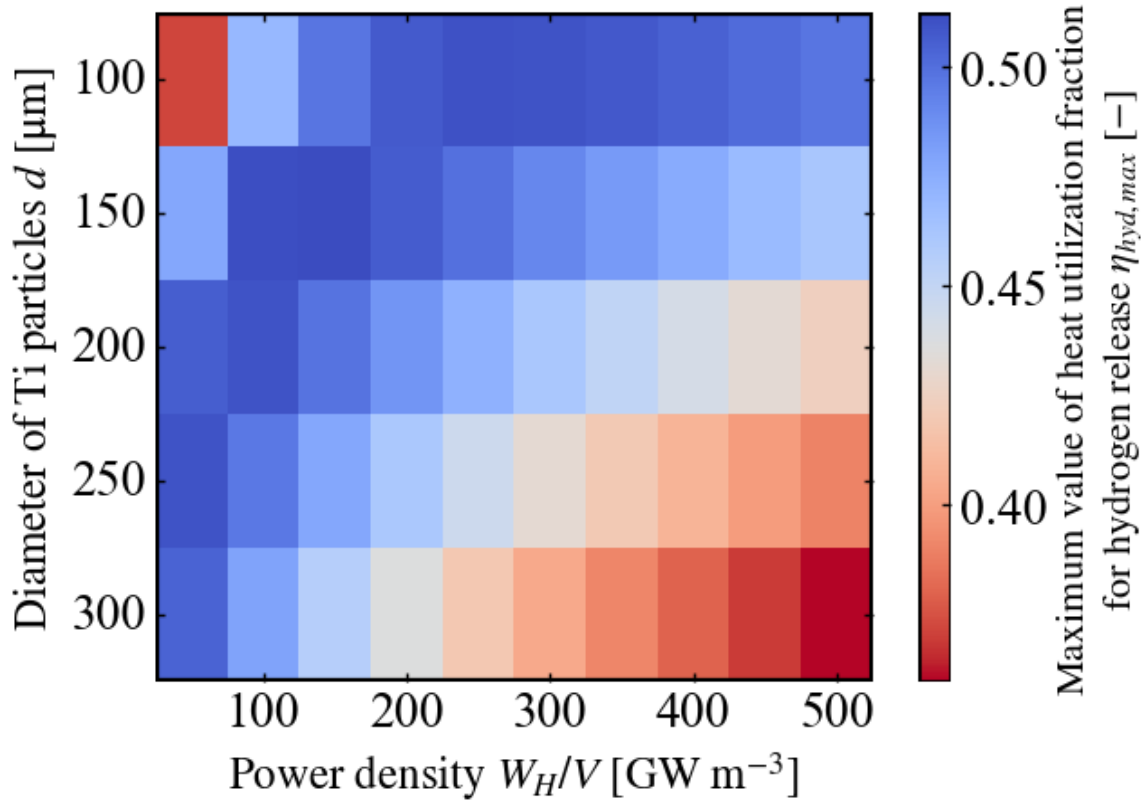


Fig. 8. $\eta_{hyd,max}$ for each condition of $d = 100, 150, 200, 250, 300 \mu\text{m}$ and $W_H/V = 50, 100, \dots, 450, 500 \text{ GW m}^{-3}$ when a magnetic field is applied to Ti particles with $T_{s0} = 25^\circ\text{C}$ and $X_0 = 1.5$ under the constant conditions of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

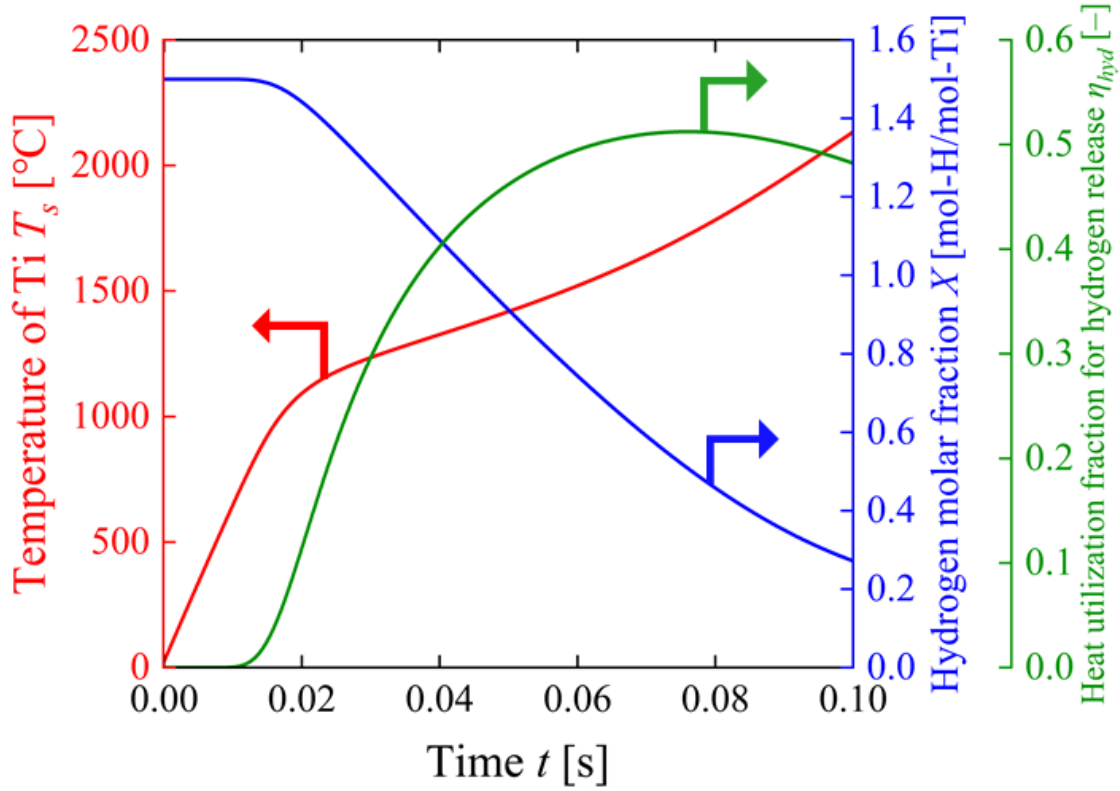


Fig. 9. Time evolution of T_s , X , and η_{hyd} in a Ti particle with $d = 150 \mu\text{m}$, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $W_H/V = 150 \text{ GW m}^{-3}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

In considering realistic operating conditions for hydrogen release from Ti particles by electromagnetic induction heating, the temperature change should be gradual to some extent from the viewpoint of safety and control. Assuming a heating time of 1 min as an example, we searched for d and W_H/V that maximize η_{hyd} after 1 min from the start of heating. The simulation conditions assumed a constant hydrogen gas atmosphere at $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$. Ti particles with different diameters with initial conditions $T_{s0} = 25^\circ\text{C}$ and $X_0 = 1.5$ were exposed to magnetic fields of different power densities for 1 min. The initial hydrogen concentration distribution within the Ti particles was assumed to be uniform, given by $C(r, 0) = X_0 N_b$. Fig. 10 presents η_{hyd} 1 min after the start of heating, denoted as

$\eta_{hyd,1min}$, for each condition of $d = 1, 2, \dots, 9, 10$ mm and $W_H/V = 50, 100, \dots, 650, 700$ MW m⁻³. Under the given conditions, applying a magnetic field with $W_H/V = 200$ MW m⁻³ to Ti particles with $d = 5$ mm results in $\eta_{hyd,1min} = 0.290$. This represents the condition with the highest $\eta_{hyd,1min}$ among all combinations of d and W_H/V . Fig. 11 shows the time evolution of T_s , X , and η_{hyd} when a magnetic field of $W_H/V = 200$ MW m⁻³ is applied to Ti particles with $d = 5$ mm, the condition that results in the maximum $\eta_{hyd,1min}$. Initially, $T_s = 25^\circ\text{C}$ and $X = 1.5$. At $t = 1$ min, $T_s = 1076^\circ\text{C}$ and $X = 0.91$. The condition is relatively mild, and it can be asserted that the search for an efficient operating condition was conducted within a range that did not cause problems from the perspectives of safety and operational control. It should be noted that the power density represents the magnitude of power consumption per unit Ti particle volume, and since the volume of one Ti particle is $V = 6.54 \times 10^{-8}$ m³ under the present condition, it is confirmed that the magnetic field strength is realistic. Also, T_s is always below the melting point of Ti, which is 1668°C . Thus, our numerical model may be a useful tool for the design of metal-based hydrogen storage systems with accelerated and energy-efficient hydrogen release by using electromagnetic induction heating. To clarify the technical novelty of our model, Table 2 compares the transfer components involved in earlier models on the transport kinetics of hydrogen in metals and the present study. By changing the parameters specific to protium and atmospheric hydrogen gas in our model to those of tritium and molten salt, respectively, potential applications in nuclear fusion reactors, as discussed in the introduction, are anticipated. In this scenario, the optimization results from this study represent the most energy-efficient operating conditions for a process in which tritium in Ti particles is recovered by electromagnetic induction heating within a molten salt blanket containing Ti particles. One notable research gap in the current study is the omission of phase transformation in Ti and the subsequent reliance on a singular set of kinetic parameters for hydrogen transport within Ti.

In addition, the assumption made regarding the direct dissipation of thermal radiation from Ti particles to outer space overlooks interparticle radiative interactions. From this viewpoint, the thermal radiation contribution in the heat balance pertaining to Ti, denoted by the fourth term on the right-hand side of Eq. (12), might be overestimated. Consequently, the heat utilization fraction for hydrogen release, η_{hyd} , may be underestimated.

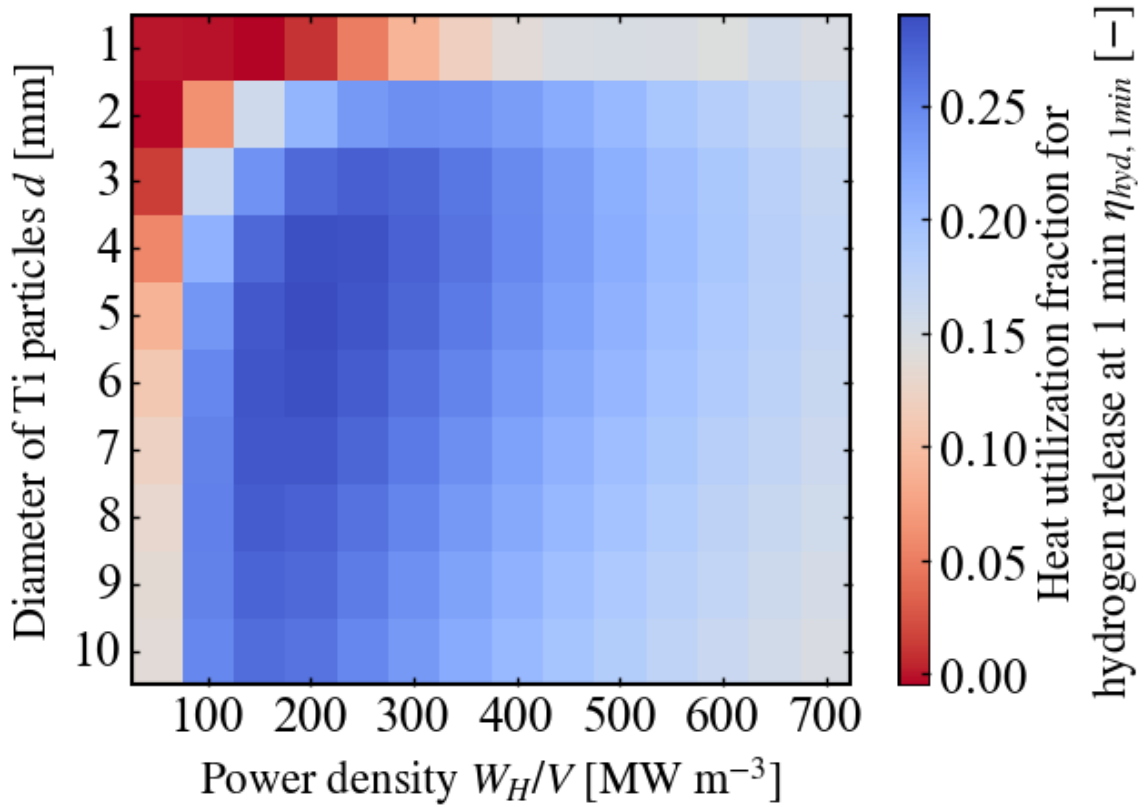


Fig. 10. η_{hyd} 1 min after the start of heating for each condition of $d = 100, 150, 200, 250, 300 \mu\text{m}$ and $W_H/V = 50, 100, \dots, 450, 500 \text{ GW m}^{-3}$ when a magnetic field is applied to Ti particles with $T_{s0} = 25^\circ\text{C}$ and $X_0 = 1.5$ under the constant conditions of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

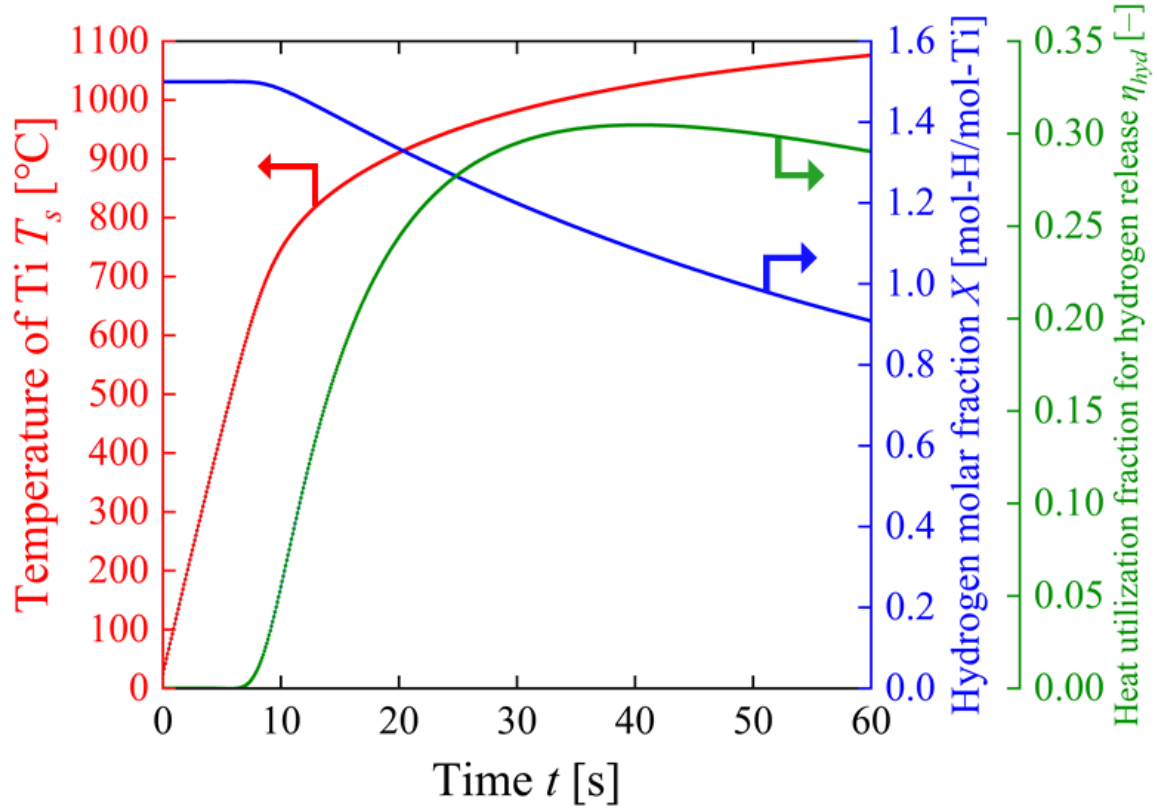


Fig. 11. Time evolution of T_s , X , and η_{hyd} in a Ti particle with $d = 5$ mm, $T_{s0} = 25^\circ\text{C}$, and $X_0 = 1.5$ when a magnetic field of $W_H/V = 200 \text{ MW m}^{-3}$ is applied to a Ti particle under the constant condition of $P_{H_2} = 0.1 \text{ atm}$ and $T_g = 25^\circ\text{C}$.

Table 2. Summary of the transfer components involved in the earlier models on the transport kinetics of hydrogen in metals and our present study.

	Electromagnetic energy	Heat	Mass
Rybakov <i>et al.</i> [42]	○		
Ignatenko <i>et al.</i> [38]	○		
Tanabe [23]	○	○	
Ward <i>et al.</i> [43]			○
Evvard <i>et al.</i> [44]			○

Nishi <i>et al.</i> ^[45]		○	○
Delaporte-Mathurin <i>et al.</i> ^[46]		○	○
This work	○	○	○

4. Conclusions

In this study, we improved our previous hydrogen transport model for Ti and developed a simulator that simultaneously calculates the temperature rise of Ti due to electromagnetic induction heating and the associated hydrogen release behavior. In our model, hydrogen transport consists of bulk diffusion, subsurface transport, and surface adsorption and desorption. Heat transport consists of electromagnetic induction heating, endotherm associated with hydrogen release, interfacial heat conduction between Ti and hydrogen gas, and thermal radiation. This induction heating scheme can be applied to achieve fast, energy-efficient hydrogen release processes in hydrogen storage in metals and tritium transfer in nuclear fusion reactors, for instance. The developed model was used to simulate the time evolution of hydrogen content in Ti particles, and we discussed important indicators for the operation of hydrogen storage in metals, such as the average hydrogen release rate and the heat utilization fraction for hydrogen release. The larger the diameter of Ti particles, the smaller the specific area, leading to a heating advantage. This facilitates hydrogen release from the perspective of temperature rise. However, as the hydrogen concentration gradient within the Ti particles decrease, hydrogen release becomes more challenging in terms of the driving force of diffusion. Therefore, there is an optimum particle size with respect to the hydrogen release rate. Additionally, a higher power density results in faster hydrogen release due to increased temperature rise, albeit at the expense of higher energy consumption. Hence, there is an optimal power density for the heat utilization fraction for hydrogen release. Our

model enables the optimization of these operational conditions for the establishment of more energy-efficient hydrogen release process. We observed that when a magnetic field with a power density of 150 W mm^{-3} based on the volume of Ti particles was applied to Ti particles with a diameter of $150 \text{ }\mu\text{m}$ for $7.6 \times 10^{-2} \text{ s}$, the heat utilization fraction for hydrogen release reached its maximum value of 0.51 under these conditions. Furthermore, by fixing the heating time at 1 min for safety and control considerations and applying a magnetic field with a power density of 200 mW mm^{-3} to Ti particles with a diameter of 5 mm, we achieved a substantial heat utilization fraction for hydrogen release, measuring 0.29. This outcome underscores the practicality of our electromagnetic–thermal–mass transport triple hybrid numerical model. By changing the parameters specific to protium and atmospheric hydrogen gas in our model to those of tritium and molten salt, respectively, potential applications in nuclear fusion reactors, as discussed in the introduction, are anticipated. In this scenario, the optimization results from this study represent the most energy-efficient operating conditions for a process in which tritium in Ti particles is recovered by electromagnetic induction heating within a molten salt blanket containing Ti particles.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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