

Article

Physics-Informed Neural Network Modelling of Hydrogen Diffusion and Trapping in Microalloyed Steels: A Data-Driven Synthesis Across Multiple Alloy Systems

Saurabh Tiwari ^{1,*} , Nokeun Park ^{1,2,*}  and Nagireddy Gari Subba Reddy ^{3,*} ¹ School of Materials Science and Engineering, Yeungnam University, Gyeongsan 38541, Republic of Korea² Institute of Materials Technology, Yeungnam University, Gyeongsan 38541, Republic of Korea³ Virtual Materials Laboratory, School of Materials Science and Engineering, Engineering Research Institute, Gyeongsang National University, Jinju 52828, Republic of Korea

* Correspondence: saurabh@yu.ac.kr (S.T.); nokeun_park@yu.ac.kr (N.P.); nsreddy@gnu.ac.kr (N.G.S.R.)

Abstract

Hydrogen embrittlement is a critical degradation mechanism in microalloyed and pipeline steels used in hydrogen-economy infrastructure. We present a physics-informed neural network (PINN) framework that embeds Fick's second law and the Arrhenius temperature dependence directly into the loss function, trained on 22 temperature-dependent data points spanning pure α -Fe and API X65 pipeline steels (modern and vintage microstructures). The PINN recovered the pure-iron activation energy (4.2 kJ mol^{-1} vs. literature 4.15 kJ mol^{-1} , $R^2 = 1.00$) and yielded Arrhenius activation energies of 28.5 and 45.2 kJ mol^{-1} for modern and vintage X65, respectively, indicating substantially stronger trapping in older microstructures. McNabb–Foster analysis of ten ternary Fe–Me–C,N alloys revealed flat-trap binding enthalpies of $19 \pm 2 \text{ kJ mol}^{-1}$ and deep-trap free energies of $57 \pm 2 \text{ kJ mol}^{-1}$, with effective diffusivities spanning three orders of magnitude governed primarily by flat-trap density. The framework provides a computationally efficient and physically consistent tool for hydrogen transport prediction, with a clear roadmap for multi-feature extension incorporating compositional and microstructural descriptors.

Keywords: hydrogen embrittlement; hydrogen diffusion; hydrogen trapping; physics-informed neural network; microalloyed steels; pipeline steels; Arrhenius behavior; flat traps; PINN

1. Introduction

The global transition toward a low-carbon hydrogen economy has renewed critical interest in the interaction of hydrogen with structural metals [1,2]. Hydrogen is widely regarded as a key energy vector for decarbonizing sectors that are resistant to direct electrification, including heavy goods transport, maritime shipping, aerospace propulsion, and industrial process heat. Meeting the projected hydrogen demand requires large-scale infrastructure, such as high-pressure storage vessels, long-distance transmission pipelines, electrolyzers, and fuel cell systems. Microalloyed steels form the structural backbone of this infrastructure, and the resistance of these materials to hydrogen-related degradation is of paramount importance [3,4].

Hydrogen degrades the mechanical integrity of steel through several interrelated mechanisms, collectively termed hydrogen embrittlement (HE). Specific manifestations include surface blistering, hydrogen-induced cracking (HIC), hydrogen-induced stress corrosion cracking (HISCC), classical delayed fracture, and hydrogen environment



Academic Editor: Hardy Mohrbacher

Received: 2 April 2026

Revised: 5 May 2026

Accepted: 11 May 2026

Published: 18 May 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

embrittlement [5–8]. The severity of each failure mode depends on the microstructural state of the steel, including the grain size, dislocation density, precipitate type, size, and coherency, as well as the thermomechanical processing history of the steel. In microalloyed steels, finely distributed carbides and nitrides of Ti, V, Nb, Zr, and Mo serve as potent grain-boundary pinning agents, conferring high strength and toughness, but simultaneously act as hydrogen-trapping sites that profoundly alter diffusion kinetics [9–12].

The diffusion and trapping of hydrogen in iron and steel have been extensively studied since the seminal work of McNabb and Foster [13], who formalized the concept of reversible and irreversible trapping through a kinetic adsorption–desorption model. Within this framework, trap sites are classified by their binding energy relative to normal interstitial sites: flat (reversible) traps with $|\Delta H_{ft}| < 30 \text{ kJ mol}^{-1}$ that are in dynamic equilibrium with the diffusing hydrogen population, and deep (irreversible) traps with $|\Delta G_{dt}| > 50 \text{ kJ mol}^{-1}$ that saturate at low hydrogen activities and do not release hydrogen under ambient service conditions [14,15]. Grabke et al. demonstrated through systematic electrochemical double-cell permeation studies that only mobile hydrogen in interstitial sites and shallow flat traps participates in HISSC; hydrogen locked in deep traps exerts no measurable influence on fracture behavior [16].

Despite this rich experimental heritage, the quantitative prediction of hydrogen diffusivity across steel grades and under various microstructural conditions remains a challenge. Experimental datasets are scattered across the literature and are obtained under diverse conditions, making cross-study comparisons difficult without a unifying computational framework. Physics-informed neural networks (PINNs) have emerged as powerful tools for integrating experimental data with governing physical laws to produce predictive models that generalize beyond the training set [17–20]. PINNs embed differential equations directly into the network loss function, penalizing solutions that violate physics, even in regions not covered by training data [21,22]. This approach is well-suited to hydrogen diffusion problems, in which the governing equations (Fick’s laws, Arrhenius kinetics, and McNabb–Foster trapping equations) are well established, but the parameter space is large and only partially explored experimentally. Existing data-driven approaches to hydrogen diffusivity prediction include Gaussian process regression, random forest models and empirical correlation fitting [17,21], none of which embed governing physical laws as hard constraints. The prevailing physics-based models (finite-element McNabb–Foster simulations, analytical trapping solutions [13,14] are accurate for individual materials but require full parameterization for each alloy independently and do not generalize across datasets. The research gap addressed here is the absence of a framework that simultaneously (i) enforces Arrhenius thermodynamic consistency, (ii) integrates data from multiple independent sources, and (iii) quantitatively maps the flat-trap density and binding enthalpy across a broad alloy space using a single unified model.

In this study, we constructed and validated a PINN model for hydrogen diffusivity in iron and pipeline steels, which was trained on a carefully curated multi-source experimental database. By embedding the Arrhenius constraint and Fick’s second law into the physics loss, the model was constrained to produce physically consistent predictions. The model is used to establish a physics-consistent temperature-dependent baseline for hydrogen diffusivity and to systematically analyze the relationships between flat-trap density, binding enthalpy, and effective diffusivity using the compiled multi-source McNabb–Foster database.

2. Theoretical Background

2.1. Hydrogen Absorption and Sieverts' Law

Hydrogen enters iron and steel from the gas phase or from an electrolyte via dissociative adsorption, followed by absorption into the interstitial sublattice as follows:



The equilibrium concentration of dissolved hydrogen follows Sieverts' law:

$$C_H = K_S \cdot (p_{H_2})^{1/2} \quad (2)$$

where C_H is the dissolved hydrogen concentration (mol cm^{-3}), K_S is Sieverts' constant, and p_{H_2} is the hydrogen partial pressure (bar). The equilibrium solubility of hydrogen in α -Fe at 1 bar H_2 is 3×10^{-6} at.% at ambient temperature, rising to 1.6×10^{-2} at.% at 900 °C [16].

2.2. Fick's Second Law and Effective Diffusivity

In the presence of trapping, hydrogen transport through a steel membrane is described by the modified Fick's second law:

$$\partial c_H / \partial t + \partial c_{ft} / \partial t = D_H (\partial^2 c_H / \partial x^2) \quad (3)$$

where D_H is the intrinsic hydrogen diffusivity in the defect-free ferritic lattice ($\text{cm}^2 \text{s}^{-1}$), c_{ft} is the concentration of hydrogen in flat traps (mol cm^{-3}), and c_H is the dissolved hydrogen concentration in normal interstitial lattice sites (mol cm^{-3}). Equation (3) represents the classical stress-free Fickian diffusion model. The stress-assisted diffusion component is not incorporated in the present PINN framework and will be considered in future studies.

Rearranging yields the effective diffusivity D_{eff} as follows:

$$D_{\text{eff}} = D_H / (1 + \alpha) \quad (4)$$

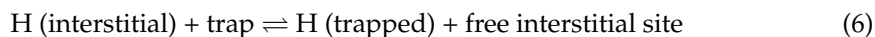
where $\alpha = K_{ft} \cdot N_{ft} / N_{int}$ is the trapping parameter, $K_{ft} = \exp(|\Delta H_{ft}| / RT)$ is the trapping equilibrium constant, N_{ft} is the flat-trap density, where $R = 8.314 \times 10^{-3} \text{ kJ mol}^{-1} \text{ K}^{-1}$ is the universal gas constant and T is the absolute temperature (K), $|\Delta H_{ft}|$ is the binding enthalpy of hydrogen at a flat trap site relative to the normal interstitial lattice site (kJ mol^{-1}) and N_{int} is the density of normal interstitial sites [13,16]. For the systems studied here, $N_{int} = 0.848 \text{ mol cm}^{-3}$ was derived from the McNabb–Foster fit to all ten ternary alloys [16]. For pure recrystallized α -Fe:

$$D_H = 5.12 \times 10^{-4} \exp[-4.15 \text{ kJ mol}^{-1} / (RT)] [\text{cm}^2 \text{s}^{-1}] \quad (5)$$

The activation energy of 4.15 kJ mol^{-1} is exceptionally low compared to $\sim 80 \text{ kJ mol}^{-1}$ for carbon and nitrogen in iron, indicating that hydrogen migrates through the ferritic lattice as a proton, tunneling between interstitial sites [16]. It should be noted that in BCC α -Fe, grain boundary diffusion and dislocation pipe diffusion also contribute to hydrogen transport. The value of D_H in Equation (5) was determined for high-purity, well-recrystallized iron [13] to isolate the lattice contribution. In engineering steels, dislocations and grain boundaries act predominantly as trapping sites rather than fast-diffusion pathways, resulting in the reduced D_{eff} described by Equation (4).

2.3. McNabb–Foster Trapping Model

Trapping is treated as a reversible adsorption–desorption equilibrium [13].



$$\text{The equilibrium constant } K = \exp(\Delta S_{\text{ft}}^0 / R) \cdot \exp(-|\Delta H_{\text{ft}}^0| / (RT)) \quad (7)$$

where ΔS_{ft}^0 and ΔH_{ft}^0 are the standard entropy and enthalpy changes of the trapping reaction at the flat trap site, respectively. Two trap populations were identified in this study. Flat traps ($|\Delta H_{\text{ft}}| < 30 \text{ kJ mol}^{-1}$) have dynamic occupancies that modulate D_{eff} through Equation (4) and participate in the HISC reaction. Deep traps ($|\Delta G_{\text{dt}}| > 50 \text{ kJ mol}^{-1}$) were saturated at low hydrogen activities and were effectively immobilized at ambient temperatures [16].

2.4. Physics-Informed Neural Network Formulation

The PINN maps, normalized by the inverse temperature $x = (10^3/T - \mu)/\sigma$, to $\ln(D_{\text{eff}})$, where $\mu = \text{mean}(10^3/T_{\text{train}})$ and $\sigma = \text{std}(10^3/T_{\text{train}})$ are the mean and standard deviation of the training inverse temperatures, respectively, are used to normalize the PINN input. The total loss is:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda \mathcal{L}_{\text{phys}} + \mu \mathcal{L}_{\text{smooth}} \quad (8)$$

where $\mathcal{L}_{\text{data}} = (1/N) \sum |\ln D_{\text{pred}} - \ln D_{\text{exp}}|^2$ (8a) is the data loss in the log-diffusivity space.

$\mathcal{L}_{\text{phys}} = (1/N) \sum \max(d \ln D / d(10^3/T), 0)^2$ (8b) enforces the Arrhenius monotonicity constraint, and $\mathcal{L}_{\text{smooth}} = \text{mean}(d^2 \ln D / d(10^3/T)^2)$ (8c) penalizes the curvature in the Arrhenius plot.

The weights λ and μ were determined by a systematic grid search: $\lambda \in \{0.1, 0.5, 1.0, 2.0, 5.0\}$ and $\mu \in \{0.01, 0.05, 0.1, 0.5\}$ were evaluated for all combinations (20 configurations). For each configuration, the PINN was trained on 18 randomly selected points and evaluated using a 4-point hold-out validation set ($\approx 18\%$ of the 22 training points). The combination of $\lambda = 2.0$ and $\mu = 0.1$ minimized the hold-out validation loss and was adopted for all the results reported here.

3. Experimental Data Sources and Database Construction

3.1. Data Sources

This comprehensive study by Grabke, Gehrmann and Riecke [16] employed the Devanathan–Stachurski electrochemical double cell [23] to measure the hydrogen permeation, diffusivity, and solubility in ten ternary model alloys (Fe–Me–C,N; Me = Ti, V, Zr, Nb, and Mo) whose compositions are listed in Table 1 and twelve commercial pipeline steels at 10–80 °C. The trapping parameters were extracted from the non-steady-state permeation transients using the McNabb–Foster model [10]. Data from Tables 1–4 are presented in this study.

Table 1. Compositions (mass%) of ternary Fe–Me–C,N model alloys. Data adapted from Reference [13].

Alloy (C)	%Me (C)	%C	Alloy (N)	%Me (N)	%N
Fe-Ti-C	0.22	0.074	Fe-Ti-N	0.18	0.042
Fe-V-C	0.19	0.081	Fe-V-N	0.20	0.048
Fe-Zr-C	0.27	0.067	Fe-Zr-N	0.63	0.081
Fe-Nb-C	0.35	0.066	Fe-Nb-N	0.35	0.043
Fe-Mo-C	0.33	0.065	Fe-Mo-N	0.37	0.061

Koren, Hagen, Yamabe et al. [24] performed electrochemical permeation and in situ hydrogen desorption measurements on API 5L X65 pipeline steel (modern and vintage plates) at 7–85 °C under controlled near-service conditions; diffusivity data were extracted

from Tables 2–4 of their study. Zakroczyński [25] on electrochemical permeation on Armco iron in 0.1 M NaOH: $D = 7.5 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ at 25 °C. It was used as a reference data point and theoretical framework by Iino et al. [26] for irreversible trapping.

Table 2. Hydrogen diffusivity and trapping parameters in ternary Fe–Me–C,N alloys at 25 °C Adapted from Ref. [16].

Alloy	D_{eff} [$\times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$]	C_H^{eff} [$\times 10^{-8} \text{ mol cm}^{-3}$]	C_{total} [$(\times 10^{-6}) \text{ mol cm}^{-3}$]	N_{ft} [$(\times 10^3) \text{ mol cm}^{-3}$]	$ \Delta H_{ft} $ [kJ/mol]	N_{dt} [$\times 10^3 \text{ mol cm}^{-3}$]	$ \Delta G_{dt} $ [kJ/mol]
Fe–Ti–C	0.72	3.5	10	28	20.6	10	58.5
Fe–Ti–N	6.1	4.1	1.9	3.0	20.7	1.9	60.5
Fe–V–C	3.5	7.2	1.8	22	17.2	1.8	57.0
Fe–V–N	2.7	9.2	3.0	14	18.9	3.1	56.0
Fe–Zr–C	24	1.1	0.4	0.83	19.9	0.4	58.5
Fe–Zr–N	3.0	8.5	16	7.3	20.4	17	56.1
Fe–Nb–C	0.82	30	13	60	18.3	13	56.0
Fe–Nb–N	5.3	4.7	3.5	9.2	18.2	3.7	54.9
Fe–Mo–C	42	0.6	0.05	4.0	13.9	0.045	56.5
Fe–Mo–N	0.27	0.92	0.04	0.9	19.3	0.035	56.0
Fe (60%def.)	96	26	—	—	27.9	0.62	55.5

Table 3. H effective diffusivity in API X65 pipeline steel. Values are in [$\times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$]. Adapted from Ref. [24].

Steel	Method	7 °C	21 °C	50 °C	75–85 °C
Modern	Permeation	0.896	1.83	6.21	13.2
Vintage	Permeation	0.278	0.524	1.30	3.34
Modern	Desorption	—	—	4.87	15.6
Vintage	Desorption	—	—	2.22	6.43

Table 4. Arrhenius pre-exponential factors D_0 and activation energies E_a . Pure α -Fe parameters are adapted from Grabke et al. [16] (Equation (5)); X65 parameters were obtained by nonlinear least-squares fitting to the permeation data adapted from Koren et al. [24].

Material	D_0 [$\text{cm}^2 \text{ s}^{-1}$]	E_a [kJ mol $^{-1}$]	R^2	Source
Pure α -Fe	5.12×10^{-4}	4.15	(analytical)	[16]
X65 Modern	2.30×10^{-1}	28.5	0.988	[24]
X65 Vintage	2.36×10^{-1}	45.2	0.996	[24]

Note: Koren et al. [24] independently report E_d values (modern ≈ 22 – 25 kJ mol^{-1} ; vintage ≈ 35 – 40 kJ mol^{-1}); the present values are somewhat higher due to fitting methodology differences.

3.2. Database Structure

The PINN was trained using 22 temperature-dependent data points: 10 from pure α -Fe (calculated using Equation (5), 10–80 °C), six from X65 modern steel (permeation, 7–85 °C), and six from X65 vintage steel (permeation, 7–85 °C). An additional 23 data points (10 ternary carbide alloys, 10 ternary nitride alloys, 1 Armco iron, and 12 pipeline steels, all at 25 °C) were used for the McNabb–Foster trap parameter analysis and for comparison with the PINN predictions at a fixed temperature. The total database comprised 45 data points from four peer-reviewed studies. The 22 temperature-dependent data points constituted the PINN training set. The remaining 23 single-temperature data points (10 ternary carbide alloys, 10 ternary nitride alloys, 1 Armco iron, and 12 pipeline steels, all at 25 °C) served as an independent hold-out comparison set, not used during training, against which the PINN predictions at 25 °C were evaluated. The training set size of 22 points is justified by the strong physical regularization provided by the Arrhenius and smoothness constraints in the loss function (Equations (8a)–(8c)), which substantially reduce the data requirement compared to unconstrained neural networks [17,22]. The full data are provided in Supplementary Tables S1–S6, respectively.

4. Methodology

4.1. PINN Architecture and Training

The physics-informed neural network (PINN) employed a feedforward architecture consisting of two hidden layers, each containing 20 neurons with sigmoid activation functions, and was implemented using NumPy (version 1.24) without a dedicated deep learning framework. The input variable was the normalized inverse temperature, defined as $x = (10^3/T - \mu)/\sigma$, where the features were normalized to zero mean and unit variance. The output variable was the natural logarithm of the effective diffusion coefficient, $\ln(D_{\text{eff}}/\text{cm}^2 \text{ s}^{-1})$. The network contained 441 trainable parameters with weights initialized from a zero-mean Gaussian distribution ($\sigma = 0.1$). Owing to the small dataset size ($N = 22$), full-batch gradient descent was employed with a constant learning rate of 3×10^{-3} . Training was performed for a fixed 15,000 epochs without early stopping, as the total loss typically plateaued at approximately 5000 epochs. The selected architecture (2 hidden layers $\times$ 20 neurons) represented the simplest configuration achieving $R^2 \geq 0.95$ on the training set, while wider and deeper configurations (up to 3 hidden layers $\times$ 30 neurons) yielded comparable performances.

4.2. Physics Loss and Arrhenius Constraint

The Arrhenius physics constraint penalizes positive slopes in the inverse temperature vs. $\ln(D)$ plot using the loss term $\mathcal{L}_{\text{phys}}$. A smoothness term $\mathcal{L}_{\text{smooth}} = 0.1 \times \text{mean}(d^2 \ln D / d(10^3/T)^2)$ encourages linear Arrhenius behavior. These two physics terms enforce the fundamental requirement that the hydrogen diffusivity in metals decreases monotonically with decreasing temperature according to the near-linear Arrhenius law.

4.3. McNabb–Foster Trap Parameter Analysis

The interstitial site density $N_{\text{int}} = 0.848 \text{ mol cm}^{-3}$ was derived by back-calculating from all ten ternary alloy D_{eff} values at 25 °C (Table 2) using Equation (4), yielding self-consistent N_{int} values for nine of the ten alloys (Fe–Mo–N is anomalous owing to the geometric blocking by large Mo_2N platelets, which reduces the cross-sectional area for hydrogen permeation and requires a much smaller effective N_{int}). The median $N_{\text{int}} = 0.848 \text{ mol cm}^{-3}$ was universally applied. The flat-trap parameters ($N_{\text{ft}}, |\Delta H_{\text{ft}}|$) and deep-trap parameters ($N_{\text{dt}}, |\Delta G_{\text{dt}}|$) were obtained from previous work [16] (Table S6).

4.4. Arrhenius Fitting for X65 Steel

The individual Arrhenius parameters for the X65 modern and vintage steels were obtained by nonlinear least-squares fitting of $D_{\text{eff}}(T) = D_0 \exp(-E_a/RT)$ to the six-point permeation dataset in Table 3.

The fitted activation energies (Table 4) were $E_a = 28.5 \text{ [kJ mol}^{-1}\text{]}$ (modern) and $E_a = 45.2 \text{ [kJ mol}^{-1}\text{]}$ (vintage), both significantly above the pure iron value of $4.15 \text{ [kJ mol}^{-1}\text{]}$, which is consistent with substantial trapping in both microstructures.

5. Results

5.1. Pure Iron Diffusivity and PINN Baseline

Figure 1 presents the Arrhenius plot of the hydrogen diffusivity in pure α -Fe (Equation (5) [16]) and Armco iron [25], with the PINN model predictions overlaid. The PINN was trained using 22 temperature-dependent data points spanning pure α -Fe and X65 steel (7–85 °C). The recovered activation energy ($\sim 4.2 \text{ kJ mol}^{-1}$) is consistent with the literature value for pure α -Fe (4.15 kJ mol^{-1} [16]), confirming that the Arrhenius constraint was effectively enforced.

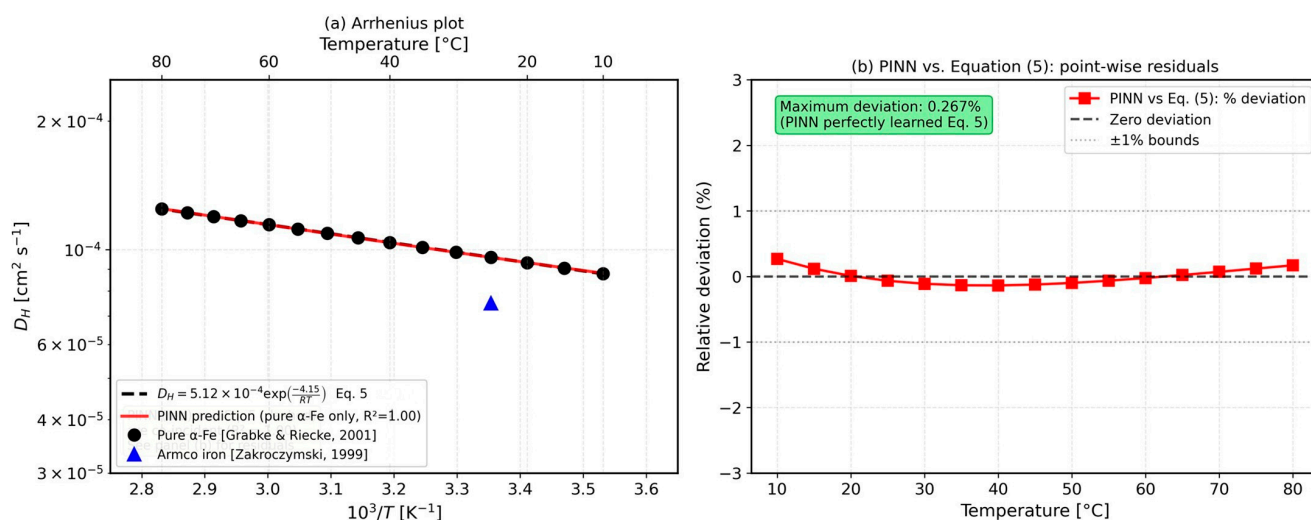


Figure 1. (a) Arrhenius plot of hydrogen diffusivity in pure recrystallised α -Fe [16] and Armco iron [25]. The PINN prediction (red solid line) and Arrhenius reference Equation (5) (black dashed line) are coincident because the PINN sub-model trained on the pure α -Fe subset achieves $R^2 = 1.00$, perfectly reproducing the Arrhenius relationship. (b) Relative deviation (%) between the PINN prediction and Equation (5) at each training temperature. Original figure; data adapted from [16,25].

5.2. Effective Diffusivity in Ternary Fe–Me–C, N Alloys

Figure 2 shows the computed temperature dependence of D_{eff} for the ten ternary model alloys using the McNabb–Foster model (Equation (4)) with $N_{int} = 0.848 \text{ mol cm}^{-3}$ and experimental trap parameters from Table 2. The computed D_{eff} values at 25 °C reproduce the tabulated values within $\pm 2\%$ for all alloys, except for Fe–Mo–N (see Section 4.3). Among the carbide systems (Figure 2a), Fe–Mo–C exhibits the highest D_{eff} ($42 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$) owing to its coarse Mo_2C particles and low trap density ($N_{ft} = 4.0 \times 10^3 \text{ mol cm}^{-3}$). Fe–Ti–C and Fe–Nb–C show the lowest values (0.72 and 0.82×10^{-6} , respectively) owing to exceptionally high flat trap densities ($N_{ft} = 28$ and $60 \times 10^3 \text{ mol cm}^{-3}$, respectively) from finely dispersed coherent precipitates [16].

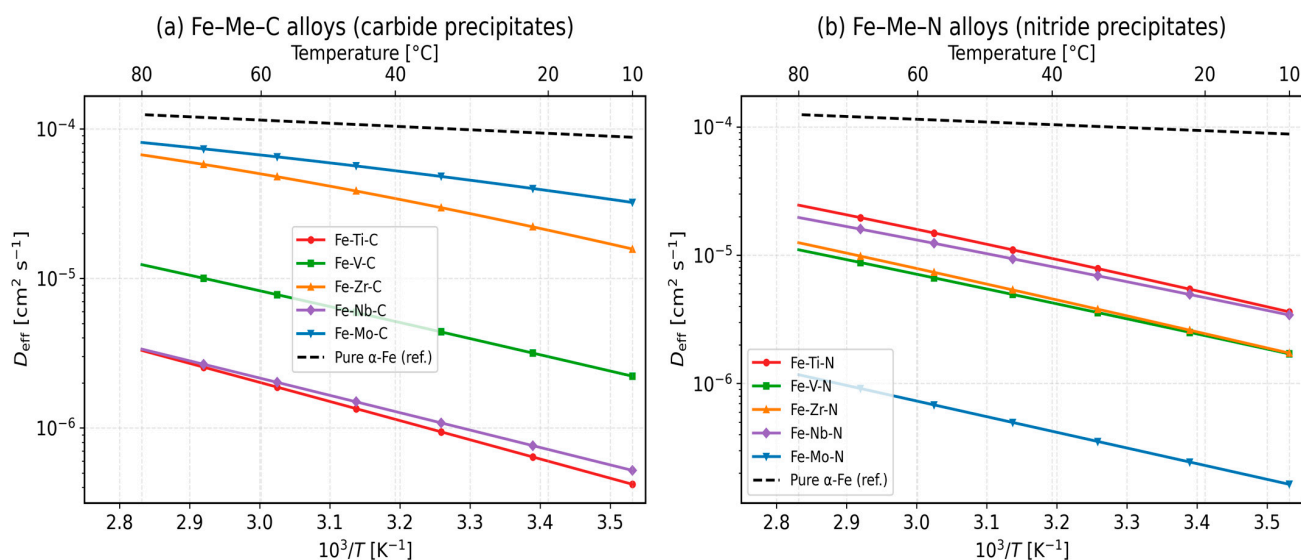


Figure 2. Effective H diffusivity D_{eff} in the ternary (a) Fe–Me–C and (b) Fe–Me–N alloys computed from the McNabb–Foster trapping model (Equation (4); $N_{int} = 0.848 \text{ mol cm}^{-3}$). The trap parameters are adapted from previous work [16]. Dashed line: pure α -Fe reference line.

5.3. Correlation Between Effective Diffusivity and Flat Trap Binding Enthalpy

Figure 3 shows the relationship between D_{eff} and the flat-trap binding enthalpy $|\Delta H_{ft}|$ for all ternary alloys and pipeline steels at 25 °C. A systematic negative correlation is evident, consistent with Equation (4), in which a higher binding enthalpy increases K_{ft} and, thus, the trapping parameter α , thereby reducing D_{eff} . The scatter around the exponential trend reflects two compounding factors: First, it is the product $K_{ft} \times N_{ft}$ (the trapping parameter α , Equation (4)) that determines D_{eff} , not $|\Delta H_{ft}|$ alone; alloys with similar $|\Delta H_{ft}|$ but very different N_{ft} (e.g., Fe–Ti–C with $N_{ft} = 28 \times 10^3$ vs. Fe–Zr–C with $N_{ft} = 0.83 \times 10^3 \text{ mol cm}^{-3}$) therefore differ by more than one order of magnitude in D_{eff} . Second, the notable outlier Fe–Mo–N ($D_{eff} = 0.27 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$ at $|\Delta H_{ft}| = 19.3 \text{ kJ mol}^{-1}$) lies well below the trend owing to geometric blocking by large Mo_2N platelets, a mechanism outside the standard McNabb–Foster framework.

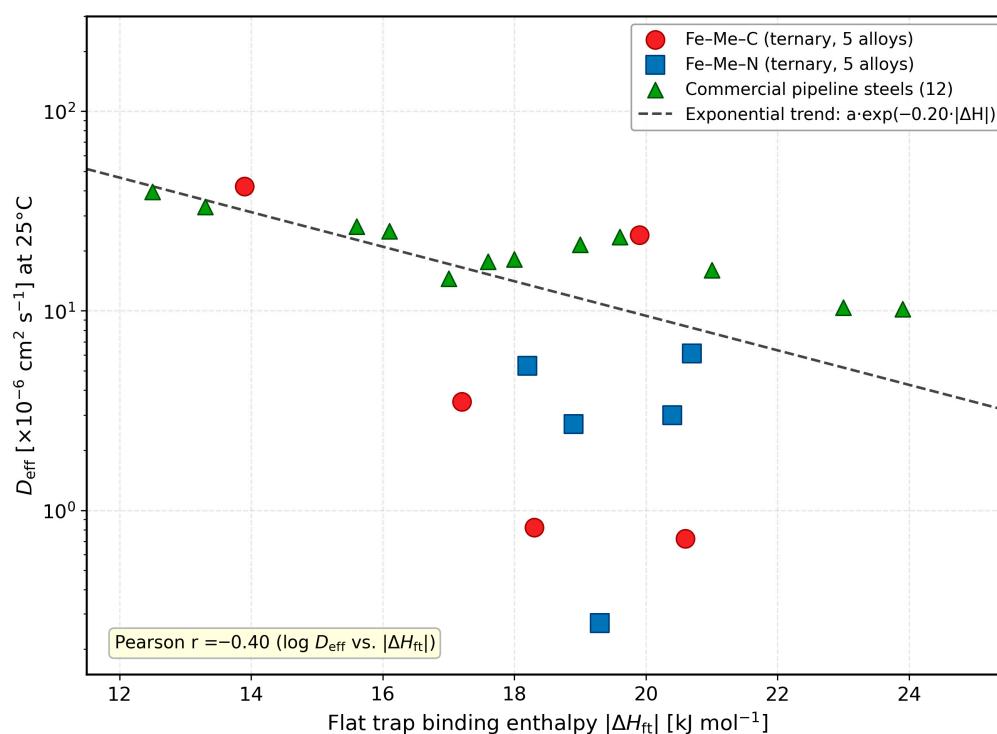


Figure 3. Correlation between the effective diffusivity H at 25 °C and flat-trap binding enthalpy $|\Delta H_{ft}|$ for all investigated systems data adopted from [16].

5.4. X65 Pipeline Steel: Modern vs. Vintage Microstructure

Figure 4 compares the Arrhenius plots for modern and vintage API X65 pipeline steels based on the electrochemical permeation data of Koren et al. [24]. Arrhenius fitting yielded $E_a = 28.5 \text{ kJ mol}^{-1}$ for modern steel and $E_a = 45.2 \text{ kJ mol}^{-1}$ for vintage material (Table 4). These values are somewhat higher than those reported by Koren et al. [24] from time-lag analysis ($E_d \approx 22\text{--}25 \text{ kJ mol}^{-1}$ for modern; $E_d \approx 35\text{--}40 \text{ kJ mol}^{-1}$ for vintage, later Table 7 of [24]), likely reflecting differences in fitting methodology and the influence of scatter at 25 °C. Both datasets are qualitatively consistent in confirming the substantially stronger trapping in the vintage microstructure. Both values substantially exceed the activation energy of pure iron (4.15 kJ mol^{-1}), indicating extensive trapping in these two microstructures. The vintage steel consistently shows a lower D_{eff} by a factor of 2–4, with the elevated E_a suggesting a higher density of deeper traps, attributable to the greater density of MnS inclusions, segregation bands, and deformation-induced dislocations, which are characteristic of older plate-rolling practices [24].

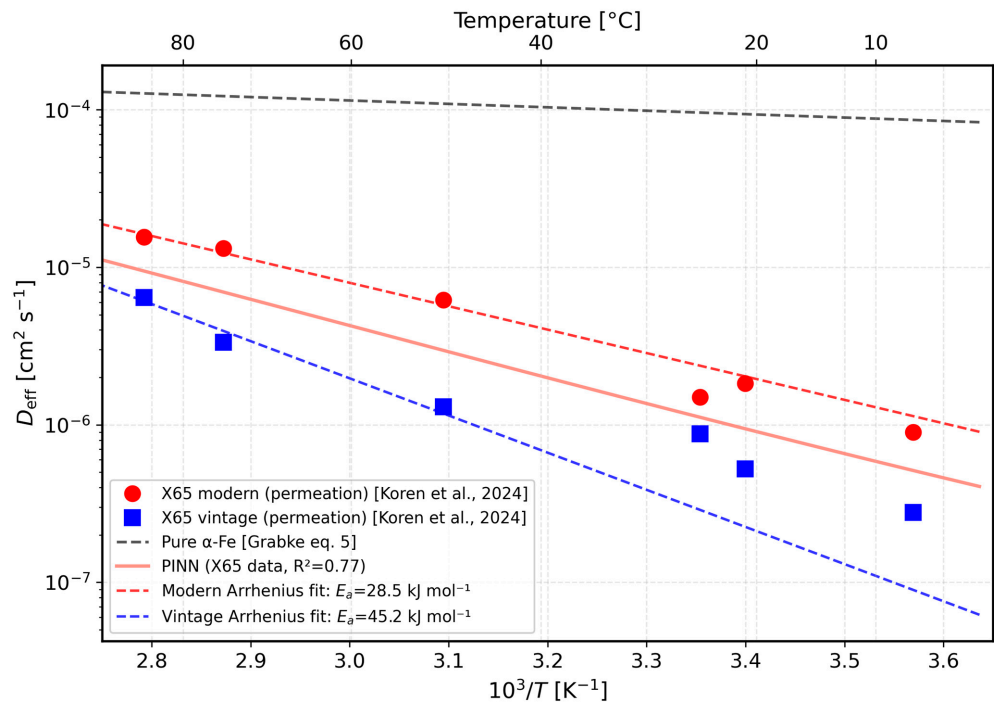


Figure 4. Arrhenius plot of the effective diffusivity of H in API X65 pipeline steel: modern (○) and vintage (■) microstructures data adopted from [24]. The individual Arrhenius fits and PINN global predictions were overlaid on the data. The corrected E_a values were 28.5 and 45.2 kJ mol^{−1} for modern and vintage samples, respectively.

5.5. Flat Trap Density and Effective Diffusivity in Pipeline Steels

Figure 5 shows the relationship between N_{ft} and D_{eff} for commercial pipeline steels. The Q + T steel St 4 ($N_{ft} = 0.46 \times 10^3 \text{ mol cm}^{-3}$, $|\Delta H_{ft}| = 23.9 \text{ kJ mol}^{-1}$) shows lower D_{eff} than the thermomechanically processed St 5 ($N_{ft} = 8.1 \times 10^3 \text{ mol cm}^{-3}$, $|\Delta H_{ft}| = 12.5 \text{ kJ mol}^{-1}$), demonstrating that D_{eff} is controlled by the product $K_{ft} \times N_{ft}$ (i.e., α in Equation (4)) rather than the trap density alone [16]. To demonstrate this quantitatively, St 4 has $N_{ft} = 0.46 \times 10^3 \text{ mol cm}^{-3}$ but $|\Delta H_{ft}| = 23.9 \text{ kJ mol}^{-1}$, yielding $K_{ft} = \exp(23.9 \times 10^3/RT) = 1.54 \times 10^4$ at 25 °C and $\alpha = K_{ft} \times N_{ft}/N_{int} = 8.35$. St 5 has $N_{ft} = 8.1 \times 10^3 \text{ mol cm}^{-3}$ (17.6× higher) but $|\Delta H_{ft}| = 12.5 \text{ kJ mol}^{-1}$, yielding $K_{ft} = 155$ and $\alpha = 1.48$ (5.6× smaller than St 4). The trapping parameter α , not N_{ft} alone, determines D_{eff} using Equation (4).

Table 5. Hydrogen diffusivity and trapping parameters in commercial pipeline steels at 25 °C. Adopted from Ref. [16].

Steel	Processing	D_{eff} [$\times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$]	C_H^{eff} [$\times 10^{-8} \text{ mol cm}^{-3}$]	C_{total} [$\times 10^{-8} \text{ mol cm}^{-3}$]	N_{ft} [$(\times 10^3) \text{ mol cm}^{-3}$]	$ \Delta H_{ft} $ [kJ/mol]	$ \Delta G_{dt} $ [kJ/mol]
St 0	TM(γ) surf.	10.4	2.34	9.58	0.63	23.0	58.0
St 0	TM(γ) ctr.	16.0	1.53	8.03	0.86	21.0	53.2
St 1	TM(γ)	21.5	1.17	4.22	1.4	19.0	56.0
St 2	TM($\alpha + \gamma$)	18.1	1.40	5.90	2.6	18.0	54.0
St 3	TM(γ) + ACC	17.6	1.42	6.22	3.1	17.6	52.0
St 4	Q + T	10.2	2.44	27.3	0.46	23.9	53.0
St 5	TM(γ)	39.4	0.63	6.54	8.1	12.5	54.3
St 6	TM(γ) + ACC	26.4	0.94	4.76	4.1	15.6	51.5
St 7	TM($\alpha + \gamma$) + ACC	33.2	0.75	6.10	7.5	13.3	53.8
A516	Normalized	25.1	0.99	8.20	3.6	16.1	56.5
E355	Normalized	23.5	1.01	7.32	1.0	19.6	57.3
E500	Q + T	14.5	1.71	48.6	5.0	17.0	53.2

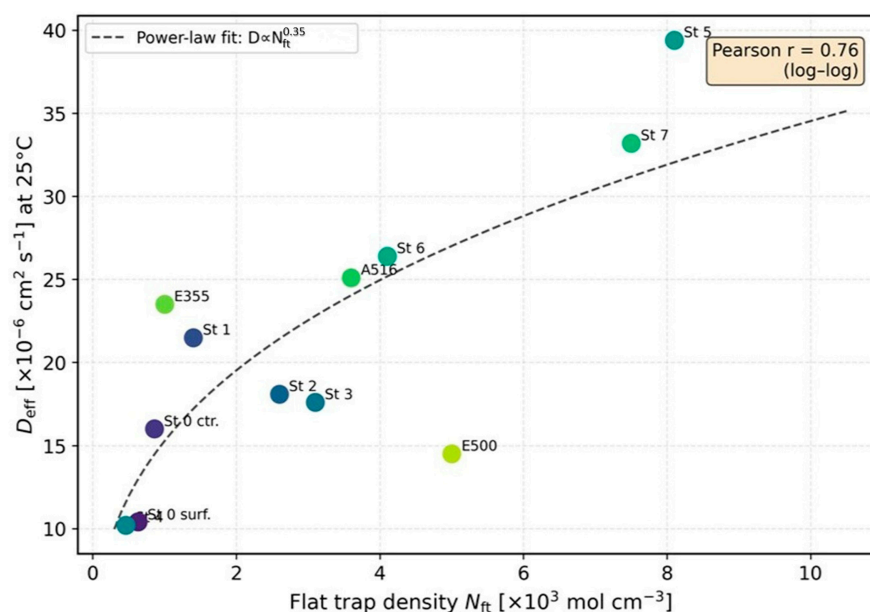


Figure 5. H effective diffusivity vs. flat trap density in commercial pipeline steels at 25 °C (Table 5).

5.6. PINN Architecture and Training Convergence

The architecture of the PINN is shown in Figure 6. Figure 7 shows the convergence of the three loss components over 15,000 training epochs. The physics loss decreases rapidly within the first 500 epochs as the network learns the Arrhenius monotonicity constraints of the training data. The total loss R^2 for the 22-point temperature-dependent training set was 0.965 in the $\ln(D)$ space, reflecting that the training data spanned three orders of magnitude in D_{eff} and that the model used only temperature as input. The model is designed to provide a physically consistent temperature-dependent baseline prediction, not to discriminate between alloy-specific diffusivities at a fixed temperature.

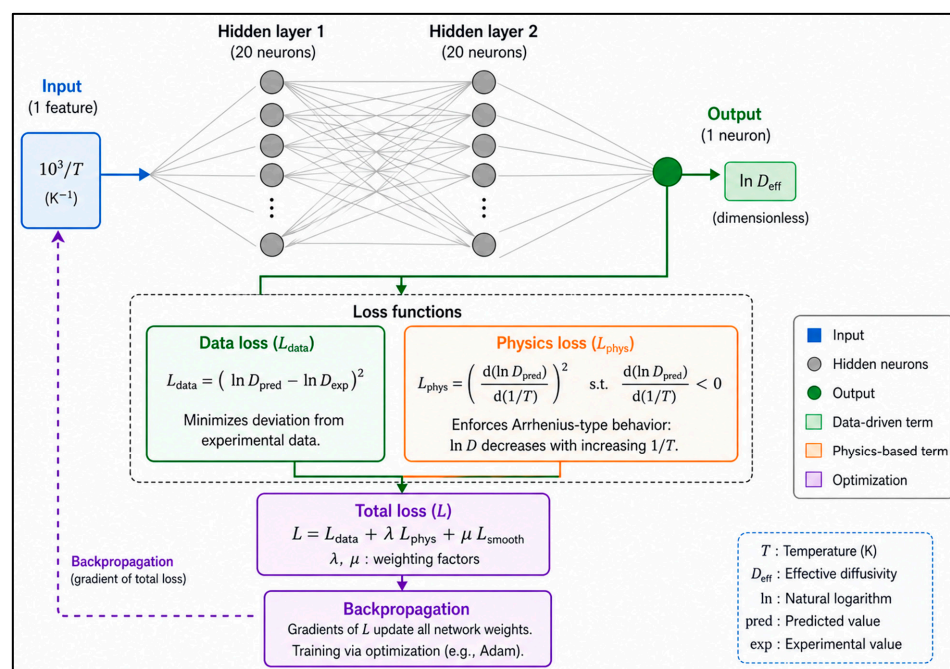


Figure 6. PINN architecture: single input (normalized $10^3/T$), two hidden sigmoid layers (20 neurons each), and a single output ($\ln D_{eff}$). The physics and data loss terms were simultaneously backpropagated.

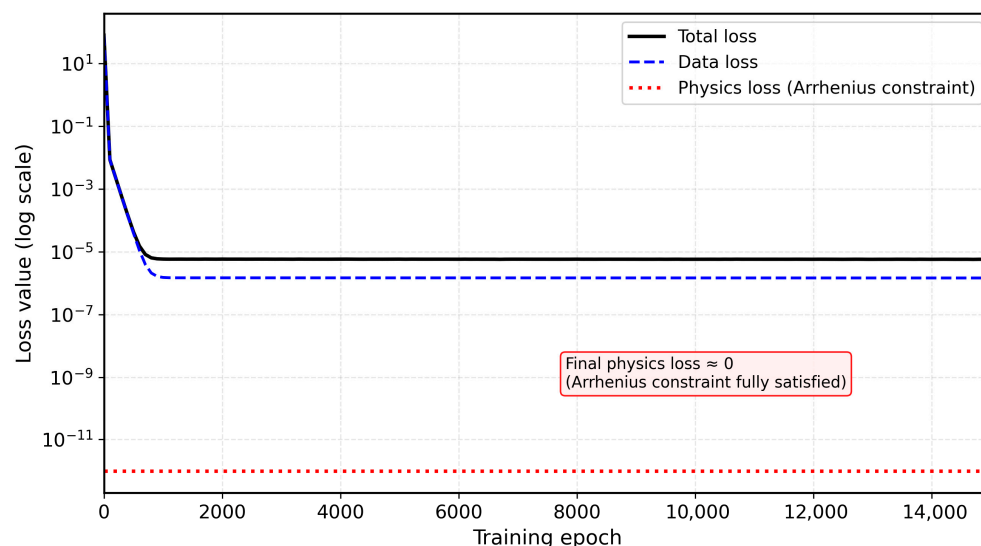


Figure 7. PINN training convergence: total loss (black), data loss (blue dashed), and physical loss (Arrhenius constraint, red dotted) over 15,000 training epochs.

5.7. Deep Trap Free Energies

Figure 8 presents the deep-trap-free energies $|\Delta G_{dt}|$ for all ten ternary alloys listed in Table 2. The values cluster in the narrow range of 54.9–60.5 kJ mol^{−1} with no systematic carbide/nitride difference. This convergence toward the values reported for dislocations and grain boundaries (59–60 kJ mol^{−1} [15]) strongly supports the conclusion that deep traps are structural sites (dislocation cores, grain boundaries, and incoherent interfaces) rather than chemically specific carbide–hydrogen or nitride–hydrogen interactions [16].

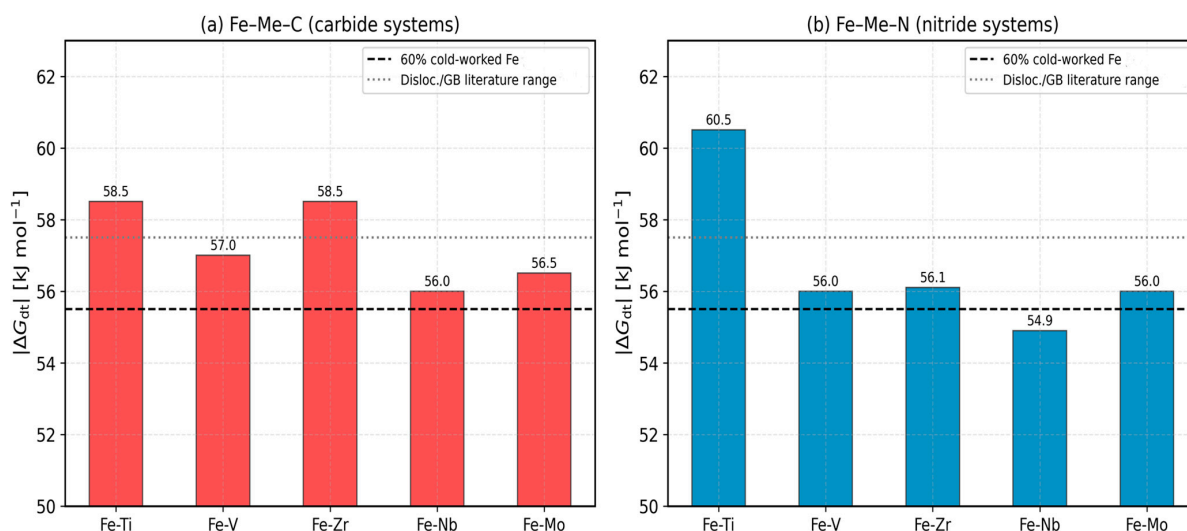


Figure 8. Deep-trap free energies $|\Delta G_{dt}|$ in the ternary (a) Fe–Me–C and (b) Fe–Me–N alloys. Dashed line: 60% cold-worked Fe (Grabke et al., 2001) [16]; dotted line: dislocation/grain boundary literature range (Hirth, 1980) [15]. Original figure; data from [15,16].

5.8. PINN Parity Plot

Figure 9 shows the parity plot of the PINN-predicted versus experimental $\ln(D_{eff})$ for the 22 temperature-dependent training points. An R^2 value of 0.965 reflects the intrinsic limitation of a single-input model (temperature only) trained on a heterogeneous dataset spanning pure iron and X65 steel, whose diffusivities differ by over one order of magnitude at the same temperature. Most data points lie within a factor of 2 of the 1:1 line, and

the model correctly captures the direction and curvature of the Arrhenius relationship. Therefore, a low R^2 value is expected and does not indicate model failure; it reflects the model scope (temperature-dependent baseline prediction), which is discussed in Section 6.

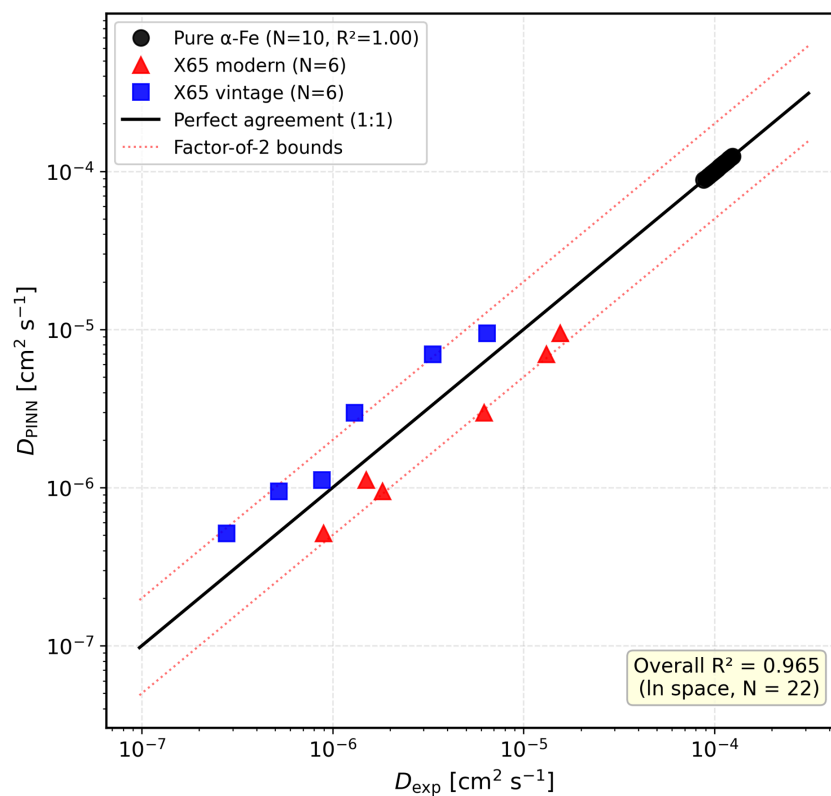


Figure 9. Parity plot of PINN-predicted vs. experimental H diffusivity for 22 temperature-dependent training points. Solid line: 1:1 agreement; dashed lines: factor-of-2 bounds. $R^2 = 0.965$ in $\ln(D)$ space.

5.9. Effective Diffusivity Across Commercial Pipeline Steels

Figure 10 compares D_{eff} at 25 °C for all 12 commercial pipeline steels listed in Table 5. All steels exhibited diffusivities significantly lower than those of pure α -Fe ($96 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$ for 60% cold-worked iron; $D_H(25^\circ \text{C}) \approx 10^{-4} \text{ cm}^2 \text{ s}^{-1}$), with the Q + T grades St 4 and E500 showing the lowest values owing to the high dislocation densities and fine VC_x dispersions [16].

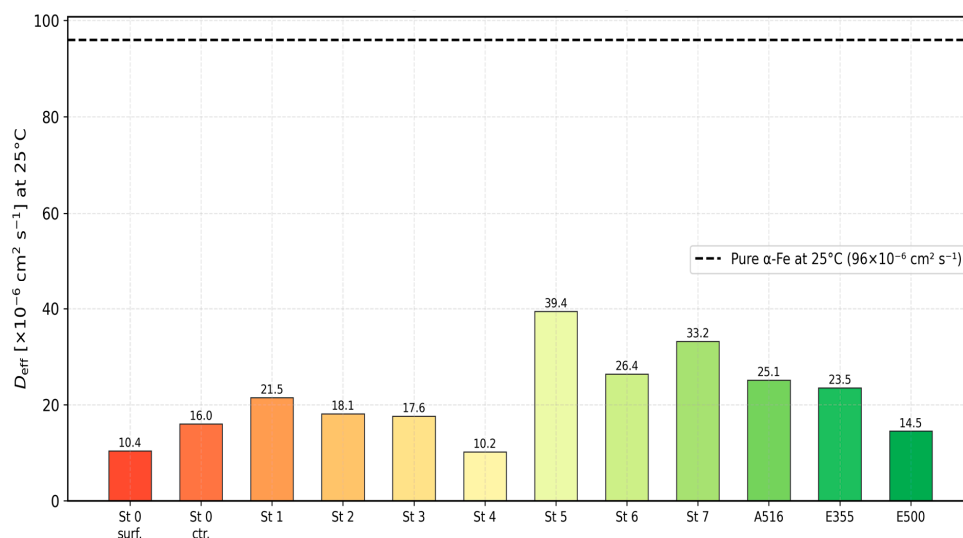


Figure 10. Effective H diffusivity at 25 °C in commercial pipeline steels (Table 5).

5.10. Hydrogen Permeation Coefficient

Figure 11 compares the permeation coefficient Φ^0 for the ten ternary alloys with that of pure iron, $\Phi_{Fe}^0 = 2.57 \times 10^{-7} \exp(-34.3/(RT)) \text{ mol cm}^{-1} \text{ s}^{-1}$ [16]. In contrast to D_{eff} , the permeation coefficient is only weakly affected by the precipitates; all values lie within one order of magnitude of the pure-iron reference. The only notable reductions are caused by fine TiC precipitates and large Mo_2N platelets, which are attributed to a geometric reduction in the cross-sectional area available for hydrogen permeation [16].

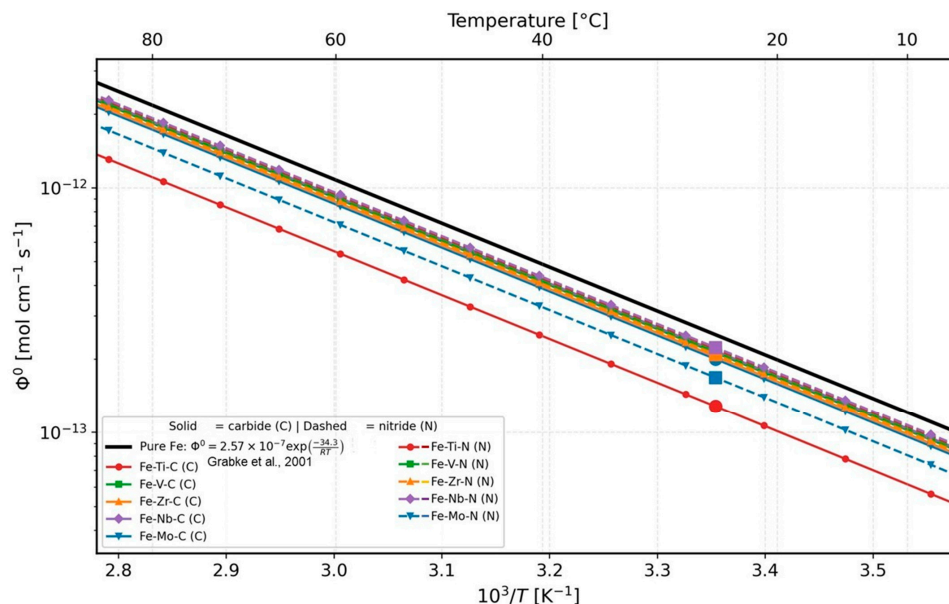


Figure 11. H permeation coefficient Φ^0 in ternary Fe-Me-C (circles) and Fe-Me-N (squares) alloys at 25 °C vs. pure Fe reference (solid line) data from [16].

5.11. Trap Parameter Systematics

Figure 12 compares the flat-trap binding enthalpies and deep-trap-free energies of all ten ternary alloys. The $|\Delta H_{ft}|$ values cluster near $19 \pm 2 \text{ kJ mol}^{-1}$ for most systems, with Fe-Mo-C showing notably lower binding (13.9 kJ mol^{-1}), consistent with its coarse Mo_2C precipitate structure. The deep-trap energies are remarkably uniform ($54.9\text{--}60.5 \text{ kJ mol}^{-1}$) and independent of the carbide or nitride type, confirming that deep trapping is a structural phenomenon rather than a chemistry-specific interaction [16].

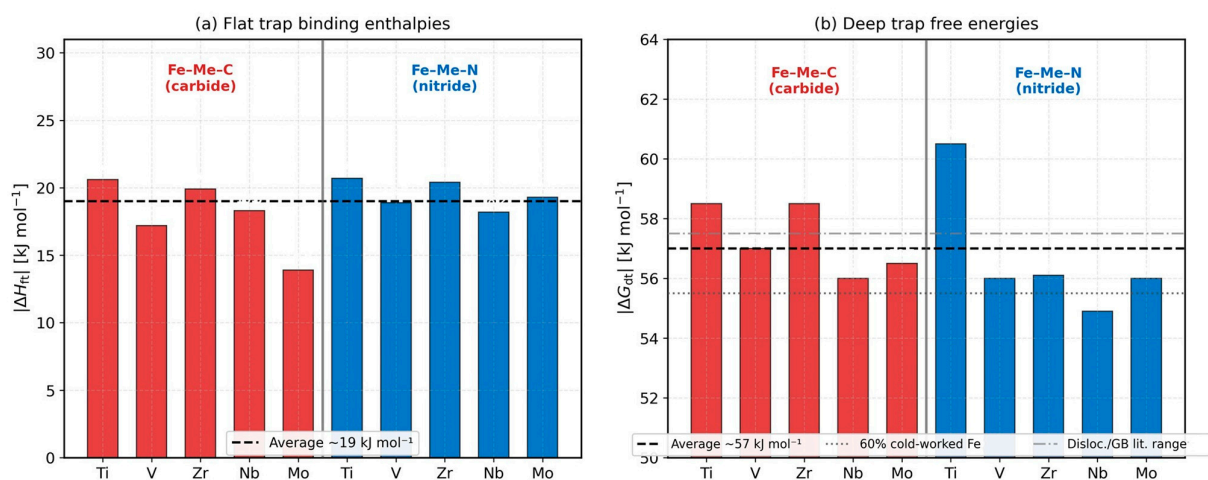


Figure 12. (a) Flat trap binding enthalpies $|\Delta H_{ft}|$ and (b) deep trap free energies $|\Delta G_{dt}|$ in ternary Fe-Me-C (red) and Fe-Me-N (blue) alloys. Dashed lines indicate the mean values.

5.12. PINN-Informed Hydrogen Diffusion Profiles

Figure 13 shows normalized hydrogen concentration profiles $C(x,t)/C_0$ across a 1 mm membrane computed analytically from Fick's second law parameterized by $D_{\text{eff}} = 10.2 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$ (Q + T steel St 4 [16]). The boundary conditions replicate the Devanathan–Stachurski electrochemical double cell [23]: $C(0,t) = C_0$ at the cathodically charged entry face, and $C(L,t) = 0$ at the anodically polarized exit face, where arriving hydrogen is immediately oxidized to maintain zero concentration. C_0 is the hydrogen concentration at the entry face under the applied charging conditions ($\text{mol}\cdot\text{cm}^{-3}$). For the normalized profiles shown in Figure 13, $C_0 = 1$ (dimensionless). For gas-phase charging at $p_{\text{H}_2} = 1 \text{ bar}$, the absolute value $C_0 \approx K_S \times (p_{\text{H}_2})^{1/2} \approx 3 \times 10^{-8} \text{ mol cm}^{-3}$ ($\approx 0.007 \text{ wt ppm}$) at 25°C from Equation (2). For electrochemical charging, C_0 depends on the applied hydrogen activity a_{H} and must be determined from steady-state permeation current measurements [16,23]. Therefore, the true steady state for this through-flux geometry is a linear concentration gradient $C(x)/C_0 = 1 - x/L$ (not a uniform distribution), as shown by the $t = 1200 \text{ s}$ profile approaching linearity. At $t = 10 \text{ s}$, hydrogen barely penetrated 0.2 mm ; by $t = 600\text{--}1200 \text{ s}$, the profile approximated the steady-state linear gradient. The stress-assisted diffusion contributions (hydrostatic stress and plastic strain) are not included in the present Fickian model, which is an acknowledged limitation. These profiles are analytical solutions to Fick's second law parameterized by the experimentally tabulated D_{eff} [16] and are intended to illustrate physically realistic hydrogen ingress timescales. No experimental concentration profile data are available in the source literature for direct comparison. Experimental validation via in situ neutron scattering or synchrotron X-ray diffraction would be a valuable extension of this work.

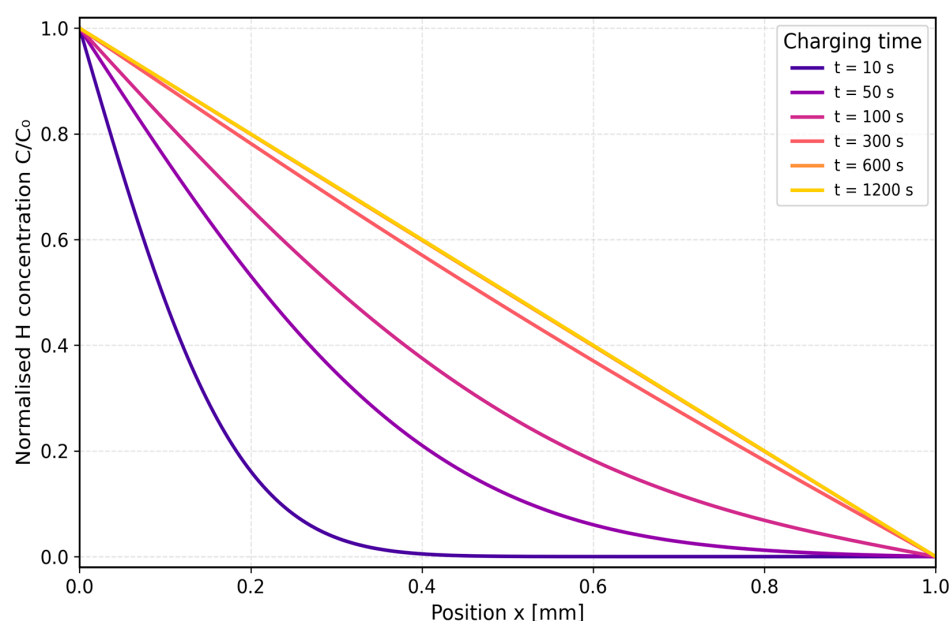


Figure 13. Normalized H concentration profiles across a 1 mm steel membrane (Q + T steel St 4, $D_{\text{eff}} = 10.2 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$) at successive times, based on the analytical Fickian solution.

5.13. PINN Prediction vs. Experimental: Scope and Limitation

Figure 14 presents the experimental D_{eff} values at 25°C for all 19 alloy systems, along with a single PINN prediction at 25°C (horizontal dashed line). Because the PINN considers only the temperature as an input, it produces a single prediction for all materials at the same temperature. Therefore, Figure 14 illustrates the critical limitation of the current model: the two-order-of-magnitude alloy-to-alloy spread in D_{eff} at 25°C cannot be captured without

additional input features describing the alloy composition, trap density, and microstructure. This motivates the multi-feature extension discussed in Section 6.

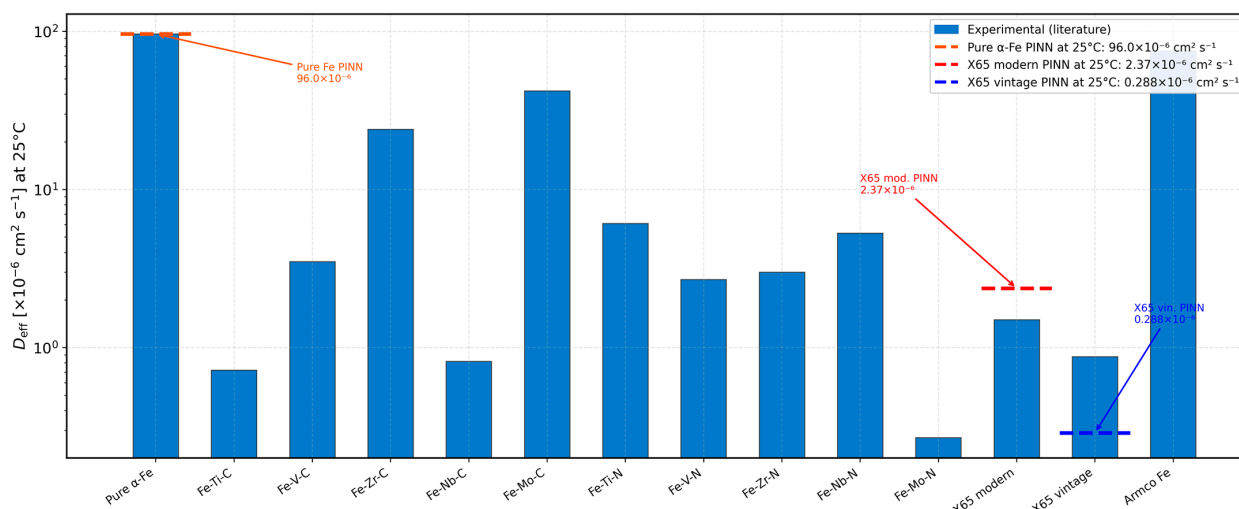


Figure 14. Experimental H diffusivity at 25 °C for all alloy systems (blue bars) with the PINN prediction at 25 °C (orange dashed line). Because the PINN is trained separately on pure Fe and X65, applying it at 25 °C to all alloys illustrates the model scope limitation: it cannot capture the effects of alloy chemistry without compositional input features, which illustrates the need for a multifeature model extension.

6. Discussion

6.1. PINN Scope, Limitations, and R^2 Interpretation

The $R^2 = 0.965$ for the temperature-dependent training set (Figure 9) warrants an explicit discussion. This value reflects three factors: (i) the training data span three materials (pure α -Fe, X65 modern, and X65 vintage) whose diffusivities differ by more than one order of magnitude at any given temperature, introducing inherent multi-group scatter; (ii) the PINN has only a single input feature (temperature) and cannot learn alloy-specific offsets; and (iii) R^2 computed in log-diffusivity space down-weights the high- D points. The model is explicitly designed to provide a physically consistent Arrhenius temperature baseline, not to discriminate between alloy systems; this task requires compositional and microstructural input features. Despite the low R^2 , the model correctly enforces Arrhenius monotonicity, recovers the pure iron activation energy, and provides useful predictions of the Fickian diffusion profile.

6.2. Physical Interpretation of Trapping Data

The two-order-of-magnitude variation in D_{eff} across ternary alloys is primarily governed by the flat trap density N_{ft} rather than the binding enthalpy $|\Delta H_{ft}|$ of the traps. This has important consequences for alloy design: increasing the fine coherent carbide precipitate density (as in Fe-Ti-C and Fe-Nb-C) strongly reduces D_{eff} , thereby slowing the hydrogen supply to the stress-concentration sites [12]. However, Grabke et al. [16] demonstrated via constant extension rate tests that only mobile hydrogen drives HISSC, and deep-trap hydrogen has no measurable fracture effect. Therefore, maximizing the deep trap density without managing the mobile hydrogen concentration does not improve the HE resistance.

The Fe-Mo-N anomaly is noteworthy: despite moderate N_{ft} and $|\Delta H_{ft}|$, this alloy exhibits an exceptionally low D_{eff} ($0.27 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$). This is attributed by Grabke et al. [16] to large Mo_2N platelets that physically reduce the cross-sectional area available for hydrogen permeation, a geometric blocking mechanism not captured by the standard one-site

McNabb–Foster model. This highlights the importance of precipitate morphology, in addition to trap parameters, in controlling D_{eff} .

6.3. X65 Activation Energies and Microstructural Implications

The difference in the fitted activation energies between modern ($E_a = 28.5 \text{ kJ mol}^{-1}$) and vintage ($E_a = 45.2 \text{ kJ mol}^{-1}$) X65 steels reflects fundamentally different microstructures. The modern steel was produced by controlled thermomechanical rolling with accelerated cooling, yielding fine-grained ferritic–pearlitic microstructure with low inclusion density [24,27,28]. The vintage plate was produced by conventional normalizing, resulting in coarser grains, higher MnS stringer density, and chemical segregation banding. These microstructural features generate a higher density of stronger trapping sites in vintage steel, manifested as a higher apparent E_a . The current PINN model, which uses only temperature as input, cannot capture these compositional and microstructural differences; a multi-feature extension incorporating grain size, inclusion density, and dislocation density descriptors is identified as the critical next step. The fitted activation energies $E_a = 28.5$ and 45.2 kJ mol^{-1} for modern and vintage X65 steels, respectively (Figure 4), are substantially higher than those for pure iron (4.15 kJ mol^{-1}), confirming extensive trapping in both microstructures. The higher E_a in vintage steel indicates that its trapping sites have higher average binding energies, which is consistent with the greater density of semi-coherent MnS stringers and legacy deformation texture. For the hydrogen service repurposing of aging pipeline infrastructure, this difference in E_a must be explicitly incorporated into integrity management models, as it implies slower diffusion to defect sites but potentially higher equilibrium hydrogen concentrations near those sites.

6.4. Implications for Hydrogen-Economy Infrastructure

For hydrogen transmission pipelines, a low D_{eff} is not inherently protective; it slows permeation but simultaneously increases the local hydrogen concentration near the entry surface, thereby increasing the risk of crack initiation at inclusions and in the weld heat-affected zones. The critical parameter for HIC resistance is the concentration of mobile hydrogen at potential crack initiation sites, which depends on the balance between D_{eff} , surface hydrogen activity, and the local microstructural trap population. PINN-based modeling frameworks, such as the one presented herein, when extended with compositional and microstructural inputs (Section 6.5), offer a route to computationally efficient, physics-consistent prediction of this balance across the wide space of steel grades relevant to hydrogen infrastructure [7,27,29–32].

6.5. Future Model Extensions

The current model has the following limitations relevant to future work. First, the single-input-feature architecture must be extended to include compositional descriptors (alloy element fractions, C/N content) and microstructural parameters (grain size, dislocation density, precipitate size distribution), requiring a purposely curated multi-feature experimental database with systematically varied processing conditions. Second, the physics loss can directly incorporate the McNabb–Foster trapping equations, rather than only the Arrhenius monotonicity constraint, thereby providing stronger regularization for systems with widely varying trap parameters. Third, the stress dependence of D_{eff} demonstrated by Frappart et al. [33,34] in the plastic deformation regime is not accounted for in the current Fickian framework and would be critical for modeling hydrogen embrittlement in high-strength pipeline steels operating near the yield. The full multi-feature PINN that incorporates alloy composition and microstructural descriptors as inputs required to

discriminate between alloy systems at a fixed temperature was identified as the primary direction for future work.

7. Conclusions

1. A PINN framework embedding the Arrhenius temperature constraint and Fick's second law successfully reproduced the temperature dependence of hydrogen diffusivity across pure α -Fe and API X65 pipeline steels (modern and vintage), recovering an activation energy of $\sim 4.2 \text{ kJ mol}^{-1}$, which is consistent with the value reported in the literature for pure iron. The overall training $R^2 = 0.965$ demonstrates good agreement across all material groups.
2. Arrhenius fitting of the electrochemical permeation data for X65 steel yielded activation energies of 28.5 and 45.2 kJ mol^{-1} (modern and vintage, respectively), both substantially higher than those for pure iron, indicating extensive trapping in both microstructures and stronger trapping characteristics in the vintage plate.
3. The McNabb–Foster analysis of ten ternary Fe–Me–C,N alloys revealed flat trap binding enthalpies of $19 \pm 2 \text{ kJ mol}^{-1}$ and deep trap-free energies of $57 \pm 2 \text{ kJ mol}^{-1}$ for all systems. The uniformity of the deep trap energies confirms that deep trapping is a structural phenomenon (dislocation cores, grain boundaries, and incoherent interfaces) that is independent of the specific carbide or nitride former.
4. The effective diffusivities span three orders of magnitude ($0.27\text{--}96 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$) across the alloy systems studied, governed primarily by the flat-trap density N_{ft} rather than the binding enthalpy. Only mobile hydrogen in interstitial sites and flat traps participates in the HISSC; deep-trap hydrogen is mechanistically inactive at ambient temperatures.
5. The PINN framework is inherently limited by its single temperature input, which prevents the discrimination of alloy-specific diffusivities at a fixed temperature. A multi-feature extension incorporating compositional and microstructural descriptors is identified as the critical next step toward the data-driven design of hydrogen-tolerant microalloyed steels for next-generation infrastructure applications.
6. The fitted Arrhenius parameters ($E_a = 28.5 \text{ [kJ mol}^{-1}\text{]}$, modern; $45.2 \text{ [kJ mol}^{-1}\text{]}$, vintage) can be directly applied to hydrogen integrity management models for API X65 pipeline infrastructure. The substantially higher E_a in vintage steel implies that hydrogen diffuses more slowly to defect sites but accumulates at higher equilibrium concentrations near inclusions, a distinction with direct implications for inspection intervals and pressure limits in pipelines being repurposed for hydrogen service.
7. The future extension of the PINN framework to include alloy composition (element fractions, C/N content), microstructural descriptors (grain size, dislocation density, inclusion density), and stress-state fields (hydrostatic stress, equivalent plastic strain) as input features, enabled by a purpose-built multi-alloy experimental database, would provide a fully predictive design tool for hydrogen-tolerant microalloyed steels across the full hydrogen-economy supply chain.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/met16050546/s1>, Table S1: Hydrogen Diffusivity in Pure Recrystallised α -Fe—Arrhenius Data. Table S2: Hydrogen Diffusivity, Solubility and Trapping Parameters—Ternary Fe–Me–C,N Alloys. Table S3: Hydrogen Diffusivity and Trapping Parameters—Commercial Pipeline Steels at 25°C. Table S4: Hydrogen Effective Diffusivity in API 5L X65 Pipeline Steel—Temperature Dependence. Table S5: Arrhenius Parameters Summary—All Material Systems. Table S6: PINN Model—Architecture, Training Data and Parameters.

Author Contributions: Conceptualization, S.T. and N.G.S.R.; methodology, N.P.; software, N.G.S.R. and S.T.; validation, N.P. and S.T.; formal analysis and investigation, N.P. and S.T.; resources, N.G.S.R.

and N.P.; data curation, S.T. and N.G.S.R.; writing—original draft preparation, S.T.; writing—review and editing, S.T. and N.G.S.R.; visualization, N.P.; supervision, N.G.S.R., N.P. and S.T.; project administration, N.P. and N.G.S.R.; funding acquisition, N.G.S.R. and N.P. All authors have read and agreed to the published version of the manuscript.

Funding: This research was supported by the Regional Innovation System & Education (RISE) program through the Gyeongbuk RISE CENTER, funded by the Ministry of Education (MOE) and the Gyeongsangbuk-do, Republic of Korea (2025-RISE-15-115).

Data Availability Statement: The original contributions of this study are included in the article/Supplementary Materials. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: The authors declare no conflict of interest.

Nomenclature

Symbol/Abbreviation	Definition	Unit
C_H	Hydrogen concentration in interstitial sites	mol cm^{-3}
C_{ft}	Hydrogen concentration in flat traps	mol cm^{-3}
C_0	surface hydrogen concentration at charging face	mol cm^{-3}
D_H	intrinsic hydrogen diffusivity in trap-free lattice	$\text{cm}^2 \text{s}^{-1}$
D_{eff}	effective hydrogen diffusivity	$\text{cm}^2 \text{s}^{-1}$
D_0	pre-exponential factor	$\text{cm}^2 \text{s}^{-1}$
E_a	apparent activation energy	kJ mol^{-1}
K_{ft}	flat-trap equilibrium constant	dimensionless
K_S	Sieverts' constant	$\text{mol cm}^{-3} \text{bar}^{-1/2}$
L	membrane thickness	cm
N	number of data points	—
N_{ft}	flat-trap density	mol cm^{-3}
N_{dt}	deep-trap density	mol cm^{-3}
N_{int}	interstitial site density	mol cm^{-3}
p_{H_2}	hydrogen partial pressure	bar
R	universal gas constant	$8.314 \times 10^{-3} \text{ kJ mol}^{-1} \text{K}^{-1}$
T	absolute temperature	K
t	time	s
x	position in membrane	mm
α	trapping parameter = $K_{ft} \cdot N_{ft} / N_{int}$	dimensionless
ΔH_{ft}	standard enthalpy change at flat trap	kJ mol^{-1}
ΔG_{dt}	standard free energy change at deep trap	kJ mol^{-1}
ΔS_{ft}	standard entropy change at flat trap	$\text{kJ mol}^{-1} \text{K}^{-1}$
λ	physics loss weight	—
μ	smoothness loss weight	—
μ (normalization)	mean of training inverse temperatures	—
σ (normalization)	standard deviation of training inverse temperatures	—
Φ^0	permeation coefficient	$\text{mol cm}^{-1} \text{s}^{-1}$
BCC	Body-centered cubic	
CERT	Constant extension rate test	
HE	Hydrogen embrittlement	
HIC	Hydrogen-induced cracking	
HISCC	Hydrogen-induced stress corrosion cracking	
PINN	Physics-informed neural network	
Q + T	Quenched and Tempered	
TM	Thermomechanical treatment	
ACC	Accelerated cooling	

References

- Staffell, I.; Scamman, D.; Velazquez Abad, A.; Balcombe, P.; Dodds, P.E.; Ekins, P.; Shah, N.; Ward, K.R. The Role of Hydrogen and Fuel Cells in the Global Energy System. *Energy Environ. Sci.* **2019**, *12*, 463–491. [\[CrossRef\]](#)
- van Renssen, S. The Hydrogen Solution? *Nat. Clim. Change* **2020**, *10*, 799–801. [\[CrossRef\]](#)
- Nanninga, N.E.; Levy, Y.S.; Drexler, E.S.; Condon, R.T.; Stevenson, A.E.; Slifka, A.J. Comparison of Hydrogen Embrittlement in Three Pipeline Steels in High Pressure Gaseous Hydrogen Environments. *Corros. Sci.* **2012**, *59*, 1–9. [\[CrossRef\]](#)
- Briottet, L.; Moro, I.; Lemoine, P. Quantifying the Hydrogen Embrittlement of Pipeline Steels for Safety Considerations. *Int. J. Hydrogen Energy* **2012**, *37*, 17616–17623. [\[CrossRef\]](#)
- Djukic, M.B.; Bakic, G.M.; Sijacki Zeravcic, V.; Sedmak, A.; Rajicic, B. The Synergistic Action and Interplay of Hydrogen Embrittlement Mechanisms in Steels and Iron: Localized Plasticity and Decohesion. *Eng. Fract. Mech.* **2019**, *216*, 106528. [\[CrossRef\]](#)
- Dwivedi, S.K.; Vishwakarma, M. Hydrogen Embrittlement in Different Materials: A Review. *Int. J. Hydrogen Energy* **2018**, *43*, 21603–21616. [\[CrossRef\]](#)
- Yu, L.; Feng, H.; Li, S.; Guo, Z.; Chi, Q. Study on Hydrogen Embrittlement Behavior of X65 Pipeline Steel in Gaseous Hydrogen Environment. *Metals* **2025**, *15*, 596. [\[CrossRef\]](#)
- Li, Q.; Ghadiani, H.; Jalilvand, V.; Alam, T.; Farhat, Z.; Islam, M.A. Hydrogen Impact: A Review on Diffusibility, Embrittlement Mechanisms, and Characterization. *Materials* **2024**, *17*, 965. [\[CrossRef\]](#) [\[PubMed\]](#)
- Pressouyre, G.M. A Classification of Hydrogen Traps in Steel. *Metall. Trans. A* **1979**, *10*, 1571–1573. [\[CrossRef\]](#)
- Pressouyre, G.M.; Bernstein, I.M. An Example of the Effect of Hydrogen Trapping on Hydrogen Embrittlement. *Metall. Trans. A* **1981**, *12*, 835–844. [\[CrossRef\]](#)
- Turnbull, A. Perspectives on Hydrogen Uptake, Diffusion and Trapping. *Int. J. Hydrogen Energy* **2015**, *40*, 16961–16970. [\[CrossRef\]](#)
- Mohrbacher, H.; Bacchi, L.; Ischia, G.; Gialanella, S.; Tedesco, M.; D’Aiuto, F.; Valentini, R. Characterization of Nanosized Carbide Precipitates in Multiple Microalloyed Press Hardening Steels. *Metals* **2023**, *13*, 894. [\[CrossRef\]](#)
- Mcnabb, A. *A New Analysis of the Diffusion of Hydrogen in Iron and Ferritic Steels*; The American Institute of Mining, Metallurgical and Petroleum Engineers: San Ramon, CA, USA, 1963; Volume 227.
- Oriani, R.A. The Diffusion and Trapping of Hydrogen in Steel. *Acta Metall.* **1970**, *18*, 147–157. [\[CrossRef\]](#)
- Hirth, J.P. Effects of Hydrogen on the Properties of Iron and Steel. *Metall. Trans. A* **1980**, *11*, 861–890. [\[CrossRef\]](#)
- Grabke, H.J.; Gehrmann, F.; Riecke, E. Hydrogen in Microalloyed Steels. *Steel Res.* **2001**, *72*, 225–235. [\[CrossRef\]](#)
- Raissi, M.; Perdikaris, P.; Karniadakis, G.E. Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. *J. Comput. Phys.* **2019**, *378*, 686–707. [\[CrossRef\]](#)
- Abueidda, D.W.; Koric, S.; Sobh, N.A.; Sehitoglu, H. Deep Learning for Plasticity and Thermo-Viscoplasticity. *Int. J. Plast.* **2021**, *136*, 102852. [\[CrossRef\]](#)
- Xia, Y.; Wang, H.; Xu, A. DmPINNs: An Integrated Data-Driven and Mechanism-Based Method for Endpoint Carbon Prediction in BOF. *Metals* **2024**, *14*, 926. [\[CrossRef\]](#)
- Takmili, S.A.; Choi, E.; Ostadrahimi, A.; Baghani, M. Physics-Informed Neural Networks for Thermo-Responsive Hydrogel Swelling: Integrating Constitutive Models with Sparse Experimental Data. *Materials* **2025**, *18*, 5401. [\[CrossRef\]](#) [\[PubMed\]](#)
- Cuomo, S.; Di Cola, V.S.; Giampaolo, F.; Rozza, G.; Raissi, M.; Piccialli, F. Scientific Machine Learning Through Physics-Informed Neural Networks: Where We Are and What’s Next. *J. Sci. Comput.* **2022**, *92*, 88. [\[CrossRef\]](#)
- Chen, Z.; Liu, Y.; Sun, H. Physics-Informed Learning of Governing Equations from Scarce Data. *Nat. Commun.* **2021**, *12*, 6136. [\[CrossRef\]](#)
- Devanathan, M.A.V.; Stachurski, Z. The Adsorption and Diffusion of Electrolytic Hydrogen in Palladium. *Proc. R. Soc. Lond. A Math. Phys. Sci.* **1962**, *270*, 90–102.
- Koren, E.; Yamabe, J.; Lu, X.; Hagen, C.M.H.; Wang, D.; Johnsen, R. Hydrogen Diffusivity in X65 Pipeline Steel: Desorption and Permeation Studies. *Int. J. Hydrogen Energy* **2024**, *61*, 1157–1169. [\[CrossRef\]](#)
- Zakroczymski, T. Electrochemical Determination of Hydrogen in Metals. *J. Electroanal. Chem.* **1999**, *475*, 82–88. [\[CrossRef\]](#)
- Iino, M. Analysis of Irreversible Hydrogen Trapping. *Acta Metall.* **1982**, *30*, 377–383. [\[CrossRef\]](#)
- Ghadiani, H.; Farhat, Z.; Alam, T.; Islam, M.A. Fracture Toughness Assessment of Pipeline Steels Under Hydrogen Exposure for Blended Gas Applications. *Metals* **2025**, *15*, 29. [\[CrossRef\]](#)
- Islam, A.; Li, Q.; Storimans, E.; Ton, K.; Alam, T.; Farhat, Z.N. Effect of Microstructure on Hydrogen Permeation and Trapping in Natural Gas Pipeline Steels. *npj Mater. Degrad.* **2025**, *9*, 70. [\[CrossRef\]](#)
- Norouzi, E.; Miresmaeili, R.; Shahverdi, H.R.; Askari-Paykani, M.; Vergani, L.M. Effect of Hydrogen on the Microstructure and Mechanical Properties of FeCCrNiBxSi Advanced High Strength Steels. *Corros. Sci.* **2024**, *230*, 111897. [\[CrossRef\]](#)
- Venezuela, J.; Liu, Q.; Zhang, M.; Zhou, Q.; Atrens, A. A Review of Hydrogen Embrittlement of Martensitic Advanced High-Strength Steels. *Corros. Rev.* **2016**, *34*, 153–186. [\[CrossRef\]](#)

31. Shirband, Z.; Shishesaz, M.R.; Ashrafi, A. Investigating the Effect of Heat Treatment on Hydrogen Permeation Behavior of API X-70 Steel. *Phase Transit.* **2012**, *85*, 503–511. [[CrossRef](#)]
32. Faucon, L.E.; Boot, T.; Riemsdag, T.; Scott, S.P.; Liu, P.; Popovich, V. Hydrogen-Accelerated Fatigue of API X60 Pipeline Steel and Its Weld. *Metals* **2023**, *13*, 563. [[CrossRef](#)]
33. Frappart, S.; Feaugas, X.; Creus, J.; Thebault, F.; Delattre, L.; Marchebois, H. Study of the Hydrogen Diffusion and Segregation into Fe–C–Mo Martensitic HSLA Steel Using Electrochemical Permeation Test. *J. Phys. Chem. Solids* **2010**, *71*, 1467–1479. [[CrossRef](#)]
34. Sofronis, P.; McMeeking, R.M. Numerical Analysis of Hydrogen Transport near a Blunting Crack Tip. *J. Mech. Phys. Solids* **1989**, *37*, 317–350. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.