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Estimation of hydrogen permeability parameters by the results of a ‘cascade’ penetration experiment

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Abstract. High-purity hydrogen is required for clean energy and a variety of chemical technology processes. Different alloys, which may be well-suited for use in gas-separation plants, were investigated by measuring specific hydrogen permeability. One had to estimate the parameters of diffusion and sorption to numerically model the different scenarios and experimental conditions of the material usage (including extreme ones), and identify the limiting factors. This paper presents a nonlinear model of fast hydrogen permeability in accordance with the specifics of the experiment and the parametric identification algorithm.

1. Introduction

Studies on the interaction of hydrogen isotopes with structural materials are mainly necessitated by problems in the energy industry (including hydrogen one) [1] and metal protection from hydrogen corrosion. Different alloys, which may be well-suited for use in gas-separation plants, were investigated by measuring specific hydrogen permeability. One had to estimate the parameters of diffusion and sorption to numerically model the different scenarios and experimental conditions of the material usage (including extreme ones), and identify the limiting factors. The limiting factors are diffusion processes as well as physical and chemical phenomena at the surface. The transfer parameters depend on the technological features of material batch production. It is therefore unreasonable to target at ‘tabular data’. Instead, effective algorithms of solving the inverse problem of parametric identification are necessary. The model matches the method of hydrogen permeability and takes into account only the main factors for the membrane filtering problem. This research is based on the article [2] and on the experimental data [3].

2. Mathematical model

2.1. Distributed transfer model

The sample of a structural material acts as a vacuum chamber barrier. The pressure of molecular hydrogen is built up in steps at the inlet side. The declining pressure in the input chamber and increasing pressure in the output chamber are measured.

Consider hydrogen transfer through the sample ($\ell$ is the plate thickness and $S$ is its area). The sample degassing is performed in advance. The temperature $T$ is constant throughout the experiment. The membrane is thin and the material has a high hydrogen permeability coefficient...
so we restrict ourselves to the standard diffusion equation:

$$\partial_t c(t, x) = D(T)\partial_x^2 c(t, x), \quad t > 0, \quad c(0, x) = 0, \quad x \in [0, \ell].$$

(1)

Here, $c(t, x)$ is the concentration of diffusing dissolved (atomic) hydrogen. The diffusion coefficient $D$ depends on the sample temperature $T$ in an Arrhenius way: $D = D_0 \exp\{-E_D/[RT(t)]\}$. Nonlinear boundary conditions are derived from the flux balance:

$$-\frac{dQ_{\text{in, out}}}{dt} = [2s(T)\mu(T)p_{0,\ell}(t) - b(T)c^2_{0,\ell}(t)]S = \mp SD\partial_x c|_{x=0,\ell}.$$

(2)

Here, $Q_{\text{in}}(t), Q_{\text{out}}(t)$ are the amounts of hydrogen atoms in the input chamber of volume $V_{\text{in}}$ and output chamber of volume $V_{\text{out}}$, $c_0(t) \equiv c(t, 0)$, $c_{\ell}(t) \equiv c(t, \ell)$. The identity sign is frequently used in the sense of equality by definition. The negative sign on the right side is used for the indices in $0$. Within the considered operating temperature range ($T \in [500, 800]$K) the gaseous hydrogen is in molecular form, but for consistency (considering that atomic hydrogen diffuses through the metal) we use atoms as the unit. The incident particle flux density $J_p$ is related to the pressure $p$ by the Hertz–Knudsen formula: $J_p = p/\sqrt{2\pi mkT}$ ($k$ is the Boltzmann constant, $m$ is the mass of a hydrogen molecule). In the context of the experiment it is convenient to select the following measurement units $[\ell] = \text{cm}$, $[p] = \text{Torr}$. Then we numerically obtain the dependence $J_p = \mu p$, $\mu(T) \approx 2.474 \cdot 10^{22}/\sqrt{T}$ ($[\mu] = 1\text{Hz}/(\text{Torr cm}^2\text{s})$, $[T] = \text{K}$). The processes of physical adsorption, chemisorption, dissociation of molecules into atoms, and dissolution take place on the surface. Only a small part of ‘incident’ $H$ atoms will, however, be absorbed into the membrane volume. This is taken into account by the factor $2s$. One can write $s$ (as a parameter of the model) instead of $2s$, but it is more convenient to interpret the probability factor $s$ as the fraction of absorbed $H$ atoms within the $2s$ notation. Thus, $2s\mu p$ is the resulting flux of atoms through the surface into the bulk without differentiation into more elementary stages.

Hereinafter, $J_{0,\ell} = bc^2_{0,\ell}$ are the desorption flux densities, $b$ is the desorption coefficient. If a constant saturation pressure of molecular hydrogen $p_{s} = \text{const}$ is maintained at a constant temperature $T$ on both sides of the membrane, the equilibrium concentration $c$ of the dissolved atomic diffusively mobile hydrogen is finally established. By equating the derivatives in the model (2) to zero, we get $\dot{c} \propto \sqrt{p_s}$: $\dot{c} = \Gamma \sqrt{p_s}$, $\Gamma \equiv \sqrt{2s\mu}/b$.

Let us define the experimental conditions more precisely. The volumes $V_{\text{in,out}}$ comprise several liters, the thickness of the membrane is $\ell < \text{nm}$, the area $S$ is about 1 cm$^2$, the inflow pressure $p_{0}(0)$ is within several hundreds Torr. It now remains to find the magnitudes of $Q_{\text{in}}, Q_{\text{out}}$. Within the time of transfer through the membrane gas is in the thermodynamical quasi-equilibrium, wherefore we use the formula $N = pV/(kT)$. Here, $N$ is the number of gas particles occupying the volume $V$ at the temperature $T = T_v$ and the pressure $p$ (in the SI system $[p] = \text{Pa}$, $[V] = \text{m}^3$, $[k] = \text{J/K}$). Taking into account Torr = 133.322 Pa and Pa = J/m$^3$ (formally), we get the expressions for the corresponding pressures and volumes in the conditions (2) $Q = 2N = \alpha pV/T$, $\alpha \approx 1.931 \cdot 10^{19}$. Here, $p, V, T$ are the values of the variables in the selected units (Torr, cm$^3$, K).

The membrane temperature should be taken for the kinetic constant $\mu(T)$. The gas inside the volumes $V_{\text{in,out}}$ may get heated up. During the preliminary experiment it is recommended to fill the chambers with a practically impermeable metal membrane between them with ambient gas. Then heat the tube and record the pressure rises. Within the framework of the ideal gas approximation this procedure enables estimation of the increments of the gas temperature inside the chambers. The corresponding gas temperatures are the ones to be used in the formula given for $Q$ (and the subsequent ones, only excluding the value $\mu$). The need of such a refinement arises from the characteristics of this particular experimental unit. Such an adjustment of the values of $T$ should not cause difficulties in further calculations. Besides, this procedure has relatively
2.2. Fast hydrogen permeability model

A quasi-stationary state is quickly established when the membrane is thin and the material has a sufficiently high hydrogen permeability coefficient: the traps are saturated and the diffusant concentration distribution is practically linear with respect to the thickness. Since near-to-surface concentrations cannot be measured, the Richardson approximation is usually used to analyze the penetrating flux: \( J(t) = -D \partial_x c = D \ell^{-1} [c_0(t) - c_\ell(t)] \approx J_R(t) = D \ell^{-1} \left[ \sqrt{p_0(t)} - \sqrt{p(t)} \right] \). Let us formulate the problem of modelling the concentrations \( c_{0,\ell}(t) \) using the pressures \( p_{0,\ell}(t) \) (the problem is also of interest per se) without the quasi-equilibrium simplification \( c(t) = \Gamma \sqrt{p(t)} \).

The quasi-stationary state is achieved within a time \( t_0 \), which is short compared to the total experiment time (the traps become saturated and \( \partial_x c = -[c_0(t) - c_\ell(t)]/\ell \)). So, the original model (1)–(2) can be simplified (taking into account the formula \( Q = \alpha p V/T \)):

\[
\begin{align*}
\dot{p}_{0,\ell}(t) &= \mp \beta_{0,\ell} \left[ c_0(t) - c_\ell(t) \right], \quad \beta_{0,\ell} \equiv SD \left[ \alpha V_{\text{in},\text{out}} \right]^{-1} T, \\
2 \mu p_{0,\ell}(t) - b c_{0,\ell}^2(t) &= \pm D \ell^{-1} \left[ c_0(t) - c_\ell(t) \right], \quad t \geq t_0 > 0.
\end{align*}
\]

The dimensionless normalized variables are convenient for numerical simulation:

\[
X_{0,\ell}(t) = 1 + 2 \ell c_{0,\ell}(t) b D^{-1}, \quad a_{0,\ell}(t) = 4 \ell^2 T^2 p_{0,\ell}(t) b^2 D^{-2} - 1. \tag{5}
\]

In addition, the system of equations (4) is compactly written in the form \( a_0 + 2X_\ell = X_0^2 \), \( a_\ell + 2X_0 = X_\ell^2 \). For the variable \( X \equiv X_\ell \) we obtain the incomplete quartic equation \( X^2 - a_\ell X = 4 [2X + a_0] \). The explicit expression is somewhat cumbersome and we will anyway have to numerically integrate the first equation of (3) in the form \( \dot{p}_0 = f(p_0) \). Therefore, we shall aim to derive equations for \( X_{0,\ell} \), since information about the dynamics of \( c_{0,\ell} \) is also important.

Differentiate the equations (4) with respect to time and substitute the pressure derivatives from (3). For the variables \( X_{0,\ell} \) we get the system:

\[
\begin{align*}
\dot{X}_0(t) &= -2s M_0 \left[ X_0 - X_{\ell} \right] \cdot \frac{X_\ell - V_{\text{in}}(t) V_{\text{out}}^{-1}}{X_0 X_\ell - 1}, \quad M_0 \equiv \frac{\mu ST}{\alpha V_{\text{in}}}, \\
\dot{X}_\ell(t) &= 2s M_\ell \left[ X_\ell - X_0 \right] \cdot \frac{X_0 - V_{\text{in}}^{-1}(t) V_{\text{out}}}{X_0 X_\ell - 1}, \quad M_\ell \equiv \frac{\mu ST}{\alpha V_{\text{out}}}, \quad t \geq t_0.
\end{align*}
\]

Let us formulate step-by-step the numerical algorithm of modelling the pressures \( p_{0,\ell}(t) \) (\( t \geq t_0 \)) for the current values of \( D, b, s \) coefficients.

1. We fix \( t = t_0 \): omit fast transient processes. For the variable \( X \equiv X_\ell \) we choose the root of the biquadratic polynomial \( [X^2 - a_\ell(t)]^2 - 4 [2X + a_0(t)] \). From physical considerations it follows that \( c_\ell(t_0) > c_\ell(t_0) \) and thus \( X > 1 + \sqrt{1 + a_\ell} = 1 + 2 \ell \Gamma \sqrt{p(t_0)} b D^{-1} \).

2. The system of equations \( a_0 + 2X_\ell = X_0^2 \), \( a_\ell + 2X_0 = X_\ell^2 \) \((t = t_0)\) yields the value of \( X_0(t_0) \).

3. We numerically integrate the ODE system (6), (7)\((X_0,\ell(t_0))\). The change in (5) defines the concentrations \( c_{0,\ell}(t) \), which are used to calculate the pressures \( p_{0,\ell}(t) \), \( t \geq t_0 \) from (4).

3. Numerical modelling of hydrogen permeability

Experimental practices employ various modifications of the penetration method and thermal desorption spectrometry (TDS). A successive use of various methods often causes impurities to appear on the sample surface. Experimental data are the input for the inverse problems of
parametric identification, which are sensitive to the level of error. It is therefore advisable to aggregate experiments to improve the accuracy and informative value of the measurements. We suggest the following set-up of the ‘cascade’ experiment.

A sufficiently high pressure of gaseous hydrogen gas was built up in steps at the inlet side. The penetrating flux was determined by mass-spectrometry in the vacuum maintained at the outlet side. This is a penetration method. Its advantage is a reliable determination of the diffusion coefficient by the Daines-Berrer method (based on lag time). It allows distinguishing between the bulk and the surface processes in the model, keeping in mind that surface parameters are significantly more difficult to estimate. When the steady state level of the penetrating flux is registered, we increase the inlet pressure and wait until a new steady state value is established. Using (at least) three pressure jumps at the inlet side we record the steady state flux values at the outlet side, thus determining ‘the degree of rectilinearity’ of the isotherm. Then the pumping for vacuum building is stopped and the experiment proceeds as the ‘communicating vessels’ method (this stage is described above). When pressure values become nearly equal (the sample is almost uniformly saturated with hydrogen) it is possible to turn off the heating, create the vacuum at both sides of the membrane and begin slowly reheating the sample (TDS-experiment).

3.1. Numerical modelling of the penetration experiment

The proposed model is adapted to the experimental conditions and the data range for alloys based on V group metals with high hydrogen permeability, in particular, data for vanadium alloys which are presented in [2–4]. We fix $T = 673\text{K}, \ell = 0.05\text{cm}, \mu(T) = 2.474 \times 10^{22}/\sqrt{T} \ 1_{\text{H}}/\text{cm}^2\text{s}, D = 2 \times 10^{-5}\text{cm}^2/\text{s}, \Gamma = 2 \times 10^{20} \ 1_{\text{H}}/\text{cm}^3/\sqrt{\text{Torr}}$, $\Phi = 4 \times 10^{15} 1_{\text{H}}/(\text{cm} s \sqrt{\text{Torr}})$. We set the value $s = 1.2 \times 10^{-4}$ and calculate the corresponding desorption coefficient $b = 2\mu s/t^2 = 5.7 \times 10^{-24}\text{cm}^4/\text{s}$. The input pressures $p_{i,2,3} = \{30, 50, 70\} \text{Torr}$ were built up in steps at the inlet, and maintained to achieve steady state fluxes at the outlet. The concentration at the membrane outlet side is near zero and at the inlet side a stationary concentration is quickly established (but it is lower than the equilibrium one): $\tilde{c} < \bar{c}$. Within the model we determine $\bar{c}_1$ and $\bar{c}_2$ by the formulas:

$\bar{c}_1 = \sqrt{2\mu s\tilde{p}_i b^{-1}}, 2\mu s\tilde{p}_i - b\tilde{c}^2 = \bar{J} = D\bar{c} \exp^{-1} \Rightarrow \tilde{c}_i = -a + \sqrt{a^2 + \Gamma^2 \tilde{p}_i}, a = D(2\beta\ell)^{-1}$.

Stage I. The boundary value problem of the penetration method is:

$c_i = Dc_{xx}, 0 < x < \ell, t > 0, \ c(t,0) = \tilde{c}_i, c(t,\ell) = 0, t \geq 0, \ c(0,x) = 0, x \in [0,\ell]$.

The penetrating flux is $J_1(t) = -Dc_{x\ell} = D\tilde{c}_1 \ell^{-1} \left[1+ 2\sum_{n=1}^{\infty} (-1)^n \exp \left\{ -n^2\pi^2 t/\ell^2 \right\} \right]$.

From the computational point of view it is convenient to introduce the dimensionless time $t' = Dt/\ell^2$ which is oriented at the characteristic diffusion time $\ell^2/D$. As small $t \rightarrow 0$ a singularity appears if we directly use the partial sum. So we provide another expression for $f(t') \ll 1$ (using the properties of the Jacobi theta function $(\theta_3)$):

$f(t') = 1 + 2\sum_{n=1}^{\infty} (-1)^n \exp \left\{ -n^2\pi^2 t' \right\} = \frac{2}{\sqrt{\pi} t'} \sum_{m=2n-1}^{\infty} \exp \left\{ -\frac{m^2}{4t'} \right\} (n \in \mathbb{N})$.

Stage II ($t_* \rightarrow 0 = 0$ is the new $t$ time zero, $t \geq 0$):

$c_i = Dc_{xx}, 0 < x < \ell, t > 0, \ c(t,0) = \tilde{c}_2, c(t,\ell) = 0, \ c(0,x) = \tilde{c}_1 (\ell - x) \ell^{-1}, x \in [0,\ell]$.

The penetrating flux is $J_2 = D\ell^{-1} \left[\tilde{c}_1 + (\tilde{c}_2 - \tilde{c}_1) \left[1+ 2\sum_{n=1}^{\infty} (-1)^n \exp \left\{ -n^2\pi^2 D t/\ell^2 \right\} \right] \right]$.

Stage II ends with $c(t_*,x) = \bar{c}_2 (\ell - x) \ell^{-1}$.

Stage III. The formulas are similar to the cyclic interchange $\tilde{c}_1 \rightarrow \tilde{c}_2, \tilde{c}_2 \rightarrow \tilde{c}_3$.

The result of connecting the stages into a single ‘experimental’ curve of the penetrating flux $J(t)$ (conventionally, $t = (t_1,t_1^* + t_2,t_2^* + t_3)$, $J = (J_1,J_2,J_3)$) is shown in Fig. 1.
3.2. The hydrogen penetration experiment without vacuum pumping

When the steady state permeability value is established during the penetration experiment, continuous pumping at the outlet and maintenance of constant pressure at the inlet are stopped. The aggregated experiment moves to the stage of ‘communicating vessels’: inlet pressure declines and outlet pressure grows \( (p_{0,t}(t) \text{ are measured}) \). We are so far talking about the direct problem of modelling hydrogen pressures inside the volumes \( V_{in,out} \).

The additional input data are \( S = 0.5 \text{ cm}^2 \), \( V_{in} = 1500 \text{ cm}^3 \), \( V_{out} = 2200 \text{ cm}^3 \), \( p(0) = \bar{p}_0 = \bar{p}_3 \), \( \bar{c} = \Gamma \sqrt{\bar{p}_0} \). We use here the data for \( V_{85\text{Ni}_{15}} \) alloy [3].

If we use the ODE system (6), (7) instead of the ‘full’ model (1)–(2) \( (c(0, x) = \bar{c}_3(\ell - x)/\ell) \), standard software packages will suffice, for example, Scilab (we substitute the values of the hydrogen temperature inside the chambers \( V_{in,out} \) into the expressions for \( M_{0,t} \)). To this end one should skip the initial time \( t_0 \) within several minutes until a quasi-stationary (not quasi-equilibrium) mode is established. Fig. 2 shows that there is no significant additional error during the numerical simulation. We wait until the sample is uniformly saturated (pressure values become nearly equal) before moving to the TDS experiment. In this article we confine ourselves to aggregating only two types of experiments and referencing [5] (and [6] for powder).

4. Parametric identification procedure

4.1. Determination of the lag time

The flux curve \( J_1(t) \) asymptotically moves to the stationary value \( \bar{J}_1 = D\bar{c}_1/\ell \). Hence, \( Q(t) = \int_0^t J_1(\tau) d\tau \approx \bar{J}_1[t - \ell^2/(6D)] \) \( (t \geq t_\ast = t_\ast^*) \). The intersection of the asymptote with the \( t \) axis gives so-called lag time \( \tau_0 = \ell^2/(6D) \) which allows estimating the diffusion coefficient (the Daines-Berrer method). Analytically, \( \tau_0 \approx t_* - \int_0^{t_*} J_1(\tau)\bar{J}_1^{-1}d\tau \), where \( J_1 \approx \bar{J}_1 \), \( t \geq t_* \). Note that a relative magnitude which does not require absolute values of the penetrating flux in any measurement units \( (J_1 = \text{sup } J_1(t)) \) is under the integral sign. In addition, the value \( t_0 \) does not depend on \( \bar{c}_1 \). It is usually assumed that the locally equilibrium concentration \( \bar{c}_1 = \Gamma \sqrt{\bar{p}_1} \) is quickly established at the inlet, so one can additionally estimate the solubility \( \Gamma = \sqrt{2\Delta\mu/\bar{b}} \) and the permeability \( \Phi = D\Gamma \) using the corresponding value \( \bar{J}_1 = D\bar{c}_1/\ell \). This assumption is not used in this article. We assume that according to the experimental conditions the stationary inlet concentration \( c_0(t) \approx \bar{c}_1 < \bar{c}_1 \) \( (t \geq \varepsilon, \varepsilon \ll 1) \) is considered to be quickly established given that \( c_1(t) \approx 0 \). The value of \( \bar{c}_1 \) as such is yet to be clarified. Thus, only the estimate of the diffusion coefficient \( D \) is considered reliable at this stage.

With a new zero-time reference \( (t_* \rightarrow t_0 = 0) \), integrating the expression \( J_2(t) \) we get \( \int_0^t J_2(\tau) d\tau \approx |J_2 - \bar{J}_1| \cdot [t - \ell^2/(6D)]^{-1} \), where \( \bar{J}_1 = D\bar{c}_1/\ell \), \( t \geq t_* = t_*^* \). Formally, we obtain the same expressions for the lag time and the estimate of \( D \) if we change both the zero time and
the flux baseline $\bar{J}_1$ value overstatement. There is no additional information here (about the target values of the surface parameters $b$ and $s$), but the triple penetration experiment allows to refine $D$. For the considered values of the model parameters we have $\tau_{01} \approx \tau_{02} \approx \tau_{03} \approx 20.8$ s.

4.2. Isotherm. Initial estimates of $b, s$.

In experimental practices analyze the isotherm, i.e. the curve of the steady state penetrating flux $\bar{J}$ dependence on the inlet pressure $\bar{p}$ when vacuum pumping is performed at the outlet side. If one targets at the Sieverts’ law and the (quasi)equilibrium concentration $\bar{c} = \Gamma \sqrt{\bar{p}}$ at the inlet side (hence $\bar{J} = D\bar{c}/\ell$), then it is natural to plot the dependence $\bar{J} = \bar{J}(\sqrt{\bar{p}})$.

Let us analyze the steady state flux balance equation:

$$2s\mu\bar{p} - b\bar{c}^2 = \bar{J} = D\ell^{-1} \Rightarrow \bar{c} = a\left[1 + \sqrt{1 + a^{-2}\Gamma^2\bar{p}}\right], \ a \equiv D(2\ell b)^{-1}, \ \bar{J} = D\ell^{-1} a\left[1 + \sqrt{1 + a^{-2}\Gamma^2\bar{p}}\right].$$

Asymptotic analysis shows that the dependence $\bar{J} / (\sqrt{\bar{p}})$ has a parabolic shape ($\bar{J} \propto \bar{p}$) at low $\bar{p}$:

$$a^{-2}\Gamma^2\bar{p} \equiv x^2 (x \propto \sqrt{\bar{p}}) \Rightarrow \bar{c} = a\left[1 + \sqrt{1 + x^2}\right] = a[0.5x^2 + \ldots]$$

and a straight line form at high inlet pressures $\bar{p}$: $a^{-2}\Gamma^2\bar{p} \gg 1 \Rightarrow \bar{J} = -D^2(2\ell^2 b)^{-1} + D\Gamma\ell^{-1}\sqrt{\bar{p}}$.

Using the straight-line segment of the isotherm we find $\Gamma\ell / \ell$ (the slope of the straight line) and knowing the estimate of $D$ we determine the initial approximation of the solubility coefficient $\Gamma$. From the intersection of the straight line with the ordinate axis we find $b$. Knowing the values of $\Gamma = \sqrt{2s\mu/b}$ and $b$ compute $s$ and $\Phi = D\Gamma$.

4.3. The final stage of parametric identification algorithm

The penetration method with vacuum pumping is characterized by a significant measurement error, and data on the penetrating flux are required (and this, in turn, requires a more accurate determination of the vacuum system characteristics). The model of the dissolved hydrogen concentration jump at the inlet side is not very precise either. We are brought to a conclusion that the ‘communicating vessels’ stage, where molecular hydrogen pressures are measured over a long time, is characterized by a much higher accuracy of measurements.

Thus, the first stage of the aggregated experiment is perceived as preliminary estimation of the coefficients $D, b, s$. It is essential that the solution of the inverse problem is unique, since the results obtained for thin laboratory membranes are extrapolated (recalculated) to the dimensions of real-life structures. The results are ‘fine-tuned’ by means of local variation of the preliminary values of $D, b, s$ in the fast hydrogen permeability model (the ODE system).

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