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A Numerical Method for the Diffusion Equation with Concentration-Dependent Diffusivity

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1. Introduction

The diffusion equation describes the phenomenon of mass transport driven by concentration gradients. For a one-dimensional diffusion equation with a constant diffusion coefficient, D, the solution can be readily derived in the form of an error function. However, when the diffusion coefficient is concentration-dependent, $D(c)$, an analytical solution is generally not obtainable. Such concentration dependence is frequently observed in various systems, including the formation of binary alloys and spinels.

Pelton and Etsell [1] and Blanc [2] proposed simplified analytical solutions for cases where $D(c)$ is defined as an intrinsic diffusivity proportional to a power of concentration. By employing the Boltzmann transformation and subsequent variable substitutions, Pelton and Etsell obtained a series solution for the diffusion equation under a semi-infinite medium, specifically for the form $D = D_0(c/c_0)$. Their work yielded a series solution expressed in terms of normalized distance and concentration. Blanc further extended this methodology to solve the problem for the more general form $D = D_0(c/c_0)^n$. Selected solutions are summarized in Fig. 1.

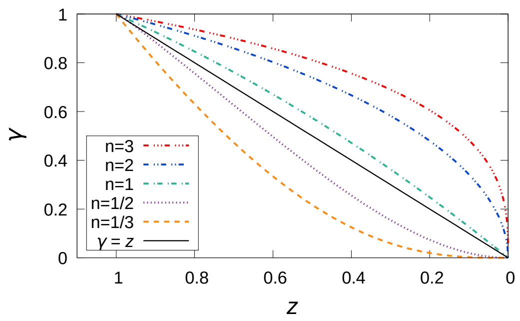

Figure 1. Plot of normalized concentration (γ) with respect to normalized distance (z)

However, previous methodologies are limited by their focus on intrinsic diffusivity, and they do not account for the extension to interdiffusion, which necessitates the consideration of two distinct diffusion coefficients. In this study, we (1) discuss the limitations of extending these analytical methods to interdiffusion systems, (2) integrate the analytical methods into a numerical approach, and (3) compare the solutions by the numerical method with intrinsic and interdiffusion cases.

2. Methods and Results

2.1. Extension to Interdiffusion

The diffusion equation is formulated using an interdiffusion coefficient based on Darken's relation, assuming intrinsic diffusivities are proportional to the power of concentration.

$$\frac{\partial c(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D(c)\frac{\partial c(x,t)}{\partial x}\right) \tag{1}$$

$$D(c) = \tilde{D}(n_A, n_B) = D_{A0}\left(\frac{c_B}{c_0}\right)^{n_A} X_B + D_{B0}\left(\frac{c_A}{c_0}\right)^{n_B} X_A \tag{2}$$

where n_A and n_B are the concentration exponents for components A and B; D_{A0} and $D_{B0}[m^2/s]$ are the constant diffusivities of pure A and B; c_A and $c_B[mol/m^3]$ are the concentrations of A and B in the A-B binary system; and c_0 is the constant total concentration where $c_0 = c_A + c_B$. Here, we assume that the diffusivity of pure B is $(\alpha+1)D_{A0}$ where α is constant.

By applying the serial transformations introduced in previous studies, the partial differential equation can be reduced to the following ordinary differential equation:

$$\begin{aligned}\frac{d^2\gamma}{dz^2} = & \frac{2y_+^2(1-z)\gamma' + (n_A+1)(1-\gamma)^{n_A}\gamma'^2}{(1-\gamma)^{n_A+1} + (\alpha+1)\gamma^{n_B+1}} \\ & - \frac{(\alpha+1)(n_B+1)\gamma^{n_B}\gamma'^2}{(1-\gamma)^{n_A+1} + (\alpha+1)\gamma^{n_B+1}}\end{aligned} \tag{3}$$

where normalized concentration is $\gamma = c_A/c_0$, normalized distance is $z = 1-(y/y_+)$, Boltzmann parameter is $y = x/(4D_0t)^{0.5}$, Boltzmann parameter at x_+ is $y_+ = x_+/(4D_0t)^{0.5}$, and x_+ is the position where $c_A = 0$; γ' denotes $d\gamma/dz$. Accordingly, the initial and boundary conditions are transformed into the boundary conditions.

$$\gamma(0) = 0, \quad \gamma(1) = 1$$

However, unlike the cases in previous research, the solution cannot be obtained by comparing the coefficients of the power series, due to the loss of the orthogonality of the power series. If we define ϕ as follows:

$$\frac{d\phi}{d\gamma} = 2y_+^2(1-z) \tag{4}$$

$$\phi = (1-\gamma)^{n_A+1}\gamma' + \alpha\gamma^{n_B+1}\gamma' \tag{5}$$

where

$$\gamma = z^{1/n_A}\sum_{m=0}^{\infty} A_m z^m + z^{1/n_B}\sum_{m=0}^{\infty} B_m z^m \tag{6}$$

and

$$\phi = z^{1/n_A}\sum_{m=0}^{\infty} C_m z^m + z^{1/n_B}\sum_{m=0}^{\infty} D_m z^m \tag{7}$$

A_m-D_m are arbitrary coefficients. Substituting Eqs. (6) and (7) into the definition of ϕ and equating the coefficients of z results in additional terms such as $z^{2/nA}$ and $z^{2/nB}$. The presence of these disparate exponents prevents a direct comparison of coefficients. Consequently, this approach cannot be analytically extended to interdiffusion systems involving two distinct concentration-dependent coefficients.

2.2. Numerical details

Having confirmed the limitations of previous analytical methodologies for interdiffusion systems, we solved the diffusion equation by integrating analytical insights with numerical techniques. Specifically, we combined the shooting method with a trial-and-error approach. Solutions were obtained numerically using a two-step iterative procedure, consisting of an inner step that determines the initial slope of the solution via the shooting method and an outer step that verifies the satisfaction of mass conservation. The shooting method transforms the boundary value problem into an initial value problem by setting the initial conditions at $z = 0$ as $\gamma(0) = \varepsilon$ and $\gamma'(0) = s$, where ε is sufficiently low and s is an initial slope. In the inner step, the ordinary differential equation is solved numerically while the parameter s is iteratively updated using Brent's method until the condition $\gamma(1) = 1$ is satisfied. Once the inner step converges, the outer step evaluates the unknown parameter y_+ using an auxiliary equation derived from mass conservation as defined below [2].

$$y_+ = \sqrt{\frac{\gamma'(1)}{2\int \gamma dz}} \tag{8}$$

The entire two-step process is repeated until the error in y_+ in the outer step falls below a tolerance of 10^{-5}, yielding the final converged solution.

2.3. Comparisons with analytic solutions

The solutions obtained via the proposed methodology were validated by comparing them with established analytical solutions. Given that the functional form of the interdiffusion coefficient in this study differs from the diffusion coefficients used in previous studies, the diffusion coefficient was modified to match the form $D = D_0(c/c_0)^n$ to facilitate a direct comparison. The modified coefficient is given as follows:

$$\tilde{D}(n_A,n_B) = D_0(\frac{c_A}{c_0})^{n_A}X_B + D_0(\frac{c_A}{c_0})^{n_B}X_A = D_0(\frac{c_A}{c_0})^n \tag{9}$$

Here, $n_A = n_B = n$ and $D_{A0} = D_{B0} = D_0$.

We compared the numerical profiles and the parameter y_+ obtained from our approach with the analytical results for various exponents ($n = 3, 2, 1, 1/2, 1/3$). Figures 2 and 3 demonstrate the comparison between the analytical and numerical solutions for two representative exponents ($n = 3$ and $1/3$), while the associated y_+ values are shown in Table 1. For solution profiles, the numerical results showed good agreement with the analytical solutions, with negligible discrepancies. For the maximum penetration distance, y_+, the relative error increases to 10% as the exponent decreases.

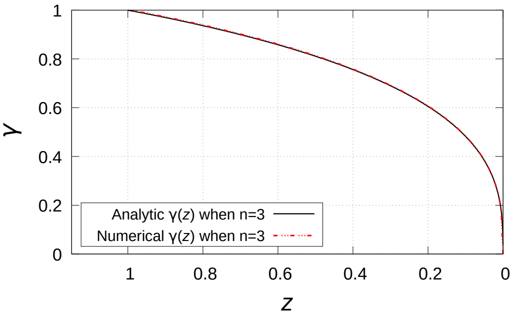

Figure 2. Comparison of analytical and numerical $\gamma - z$ plots for $n = 3$

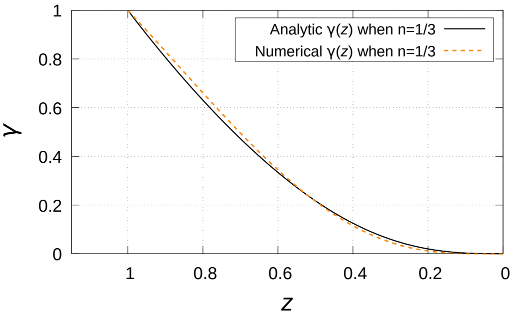

Figure 3. Comparison of analytical and numerical $\gamma - z$ plots for $n = 1/3$

Table 1. Comparison of y_+ values obtained from analytical and numerical methods

n	Numerical y_+	Analytic y_+	Error
3	0.435	0.435	$\leq 1\%$
2	0.545	0.545	$\leq 1\%$
1	0.808	0.808	$\leq 1\%$
1/2	1.216	1.204	1%
1/3	1.585	1.480	8%

2.4. Comparisons with the interdiffusion profile in nuclear waste glass

The solutions obtained via the proposed methodology were further validated by comparing them with concentration profiles in an interdiffusion system. In the interdiffusion occurring at alkali sites, the interdiffusion coefficient is typically characterized as a function of concentration. For SON68, a surrogate nuclear waste glass, the interdiffusion coefficient for Na is expressed as follows [3]:

$$\tilde{D}^{Na} = \frac{D_s^{Na} D_b^{Na}}{C_{Na} D_s^{Na} + (1 - C_{Na}) D_b^{Na}} \tag{10}$$

where $D_s^{Na}/D_b^{Na} = 2$. The interdiffusion behavior defined by Eq. (10) can be similarly simulated through the approach presented in this work. A comparison of these diffusion coefficients as a function of concentration is presented in Fig. 4. Figure 5 presents the Na diffusion profile of SON68 at 90°C for 10 days, alongside the concentration-distance plot calculated using the methodology proposed in this work. The numerical results obtained from our methodology demonstrate good agreement with the fitted experimental data.

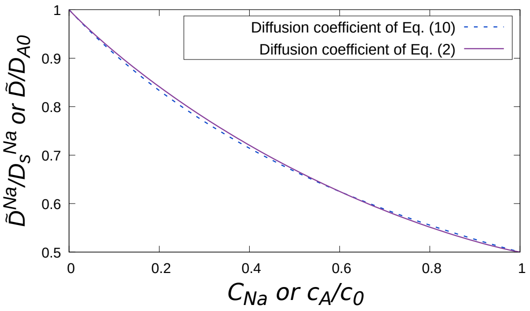

Figure 4. Comparison of diffusion coefficients. The blue dotted line follows Eq. (10) where $D_s^{Na}/D_b^{Na} = 2$. The purple line follows Eq. (2) where $n_A = 0.02$, $n_B = 0.5$ and $D_{A0}/D_{B0} = 2$ ($\alpha = -0.5$)

3. Conclusions

In this study, solutions of the diffusion equation were obtained when diffusivity is proportional to the power of the normalized concentration. We identified that extending the conventional analytical approach to interdiffusion systems leads to a fundamental limitation. The diffusion equation was transformed into an ordinary differential equation and solved using a two-step iterative procedure combining the shooting method with the trial-and-error method. The proposed method was validated by comparing it with established analytical solutions for $D = D_0(c/c_0)^n$. For cases where $n \geq 1$, the numerical results demonstrated excellent agreement with the analytical solutions, while for $n < 1$, the methodology yielded results within a reasonable error. The proposed methodology was applied to characterize the alkali interdiffusion in SON68 nuclear waste glass, showing good agreement with experimental data. Using the method proposed above, we will quantitatively analyze the characteristics of the solutions to the diffusion equation.

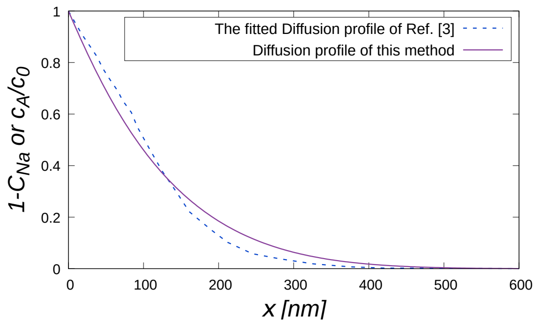

Figure 5. Comparison of diffusion profiles between SON68 Na profile at 90°C for 10 days and the diffusion profile calculated by the present method. Here, $D_s^{Na} = D_{A0}$.

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REFERENCES

[1] A. D. Pelton and T. H. Etsell, Analytical solution of Fick's second law when the diffusion coefficient varies directly as concentration, Acta Metallurgica, Vol.20, p.1269-1274, 1972.

[2] J. Blanc, Diffusion coefficients varying with a power of the concentration: Convenient solutions and a reexamination of Zn in GaAs, Journal of Applied Physics, Vol.45, p.1948-1950, 1974.

[3] J. J. Neeway, S. N. Kerisit, J. Liu, J. Zhang, Z. Zhu, B. J. Riley, and J. V. Ryan, Ion-exchange interdiffusion model with potential application to long-term nuclear waste glass performance, The Journal of Physical Chemistry C, Vol.120, No.17, p.9374-9384, 2016.