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Non-linear mass transfer in boundary layers—2. Numerical investigation

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Abstract—The numerical solution of a class of problems for non-linear mass transfer in laminar diffusion boundary layers for a gas–liquid system is obtained utilizing a numerically stable continuation type shooting procedure for the numerical integration of asymptotic boundary value problems for systems of ordinary differential equations. The influence of gas solubility and non-linear effects in the gas on the hydrodynamics and the mass transfer have been studied. Numerical results are also reported.

INTRODUCTION

In Part 1 of this study [1] an asymptotic theory was developed allowing for the calculation of the rates of mass transfer in the diffusion boundary layers close to the moving phase boundary of a gas–liquid system and accounting for the non-linear effects induced by an intensive interphase mass transfer. Comparison of these effects in the two phases by means of θ_3 and θ_4

$$\frac{\theta_3}{\theta_4} = \frac{2\rho_0\varepsilon_2\chi}{\tilde{\rho}_0\varepsilon_1} \gg 1 \qquad (1)$$

indicates that they differ by more than two orders of magnitude. This means that θ_3 and θ_4 cannot be small simultaneously when real effects are to be determined.

It was shown in ref. [1] that for practically interesting cases $\theta_4 \approx 0$ while θ_3 depends on the concentration of the substance absorbed in the gas phase and it is small for low concentrations only. Thus, for moderately high and high concentrations the asymptotic theory ceases to be valid. For this reason a numerical procedure has to be developed and such a procedure will be presented in what follows. Numerical results for several values of θ_3 and χ/ε_0 will be reported and discussed.

STATEMENT OF THE PROBLEM AND THE NUMERICAL METHOD

We shall be concerned with the numerical solution of the following boundary value problem for a system of ordinary differential equations [1]:

$$\phi_1''' + \varepsilon_1^{-1}\phi_1\phi_1'' = 0, \quad \phi_1 = \phi_1(\xi_1), \quad \xi_1 > 0$$
$$\phi_2''' + 2\varepsilon_2^{-1}\phi_2\phi_2'' = 0, \quad \phi_2 = \phi_2(\xi_2), \quad \xi_2 > 0$$
$$\psi_1'' + \varepsilon_1\phi_1\psi_1' = 0, \quad \psi_1 = \psi_1(\xi_1), \quad \xi_1 > 0$$
$$\psi_2'' + 2\varepsilon_2\phi_2\psi_2' = 0, \quad \psi_2 = \psi_2(\xi_2), \quad \xi_2 > 0 \qquad (2)$$

subject to boundary conditions

$$\begin{aligned}
\phi_1(0) &= -\theta_3\psi_1'(0)\\
\phi_1'(0) &= 2\theta_1\frac{\varepsilon_2}{\varepsilon_1}\phi_2'(0)\\
\psi_1(0) &= 1-\psi_2(0)\\
\phi_1'(\infty) &= 2\varepsilon_1^{-1}\\
\psi_1(\infty) &= 0\\
\phi_2(0) &= \theta_4\psi_2'(0)\\
\phi_2''(0) &= -\tfrac{1}{2}\theta_2\left(\frac{\varepsilon_1}{\varepsilon_2}\right)^2\phi_1''(0)\\
\psi_2'(0) &= \frac{\chi}{\varepsilon_0}\psi_1'(0)\\
\phi_2'(\infty) &= \varepsilon_2^{-1}\\
\psi_2'(\infty) &= 0.
\end{aligned} \qquad (3)$$

As seen from equations (2) and (3) this system could be decoupled into two separate boundary value problems. The first one comprises the first two equations from equations (2) and the first five equations from equations (3), while the second one comprises the remaining equations of equations (2) and (3).

Assuming initial guesses for $\phi_2'(0)$ and $\psi_2(0)$ and utilizing the improved continuation type shooting procedure [2] one could find approximations for $\psi_1'(0)$

Table 1

χ/ε_0	θ_3	$\phi_1(0)$	$\phi_1'(0)$	$\phi_1''(0)$
0	0	0	0.211 (0.200)	1.30
	0.1	0.0785 (0.0664)	0.215 (0.200)	1.40
	0.2	0.170 (0.133)	0.217 (0.200)	1.52
	0.3	0.280 (0.199)	0.219 (0.200)	1.66
0.1	0	0	0.215	1.30
	0.1	0.0733	0.216	1.39
	0.2	0.157	0.217	1.50
	0.3	0.254	0.219	1.63
1	0	0	0.216 (0.200)	1.30
	0.1	0.0450 (0.0416)	0.217 (0.200)	1.36
	0.2	0.0952 (0.0832)	0.218 (0.200)	1.42
	0.3	0.146 (0.125)	0.219 (0.200)	1.45
10	0	0	0.217	1.30
	0.1	0.0101	0.217	1.32
	0.2	0.202	0.217	1.33
	0.3	0.0304	0.217	1.34

and $\phi_1''(0)$. These quantities can be used in the second system and therefrom to calculate new approximations for $\psi_2(0)$ and $\phi_2'(0)$, etc. Thus, integrating iteratively the two systems one obtains on every iteration improved estimates for the unknown initial values $\phi_1(0), \phi_1'(0), \ldots, \psi_2'(0)$. If this iterative process is convergent it will yield approximations for the initial conditions mentioned and estimates for the 'computational infinities' for both phases together with estimates for the reliability of the computed solutions [2]. If $\chi/\varepsilon_0 > 1$ one has to modify slightly the iteration scheme (the third and eighth equations from equations (3) will exchange places) to suppress amplifying disturbances due to the unknown initial condition $\psi_1'(0)$.

Thus one has the following iteration schemes.

For $\chi/\varepsilon_0 \leqslant 1$:

$$\phi_1'''^{(k+1)} + \varepsilon_1^{-1}\phi_1^{(k+1)}\phi_1''^{(k+1)} = 0, \quad \xi_1 > 0$$

$$\psi_1''^{(k+1)} + \varepsilon_1\phi_1^{(k+1)}\psi_1'^{(k+1)} = 0, \quad \xi_1 > 0 \quad (4)$$

Table 2

χ/ε_0	θ_3	$\psi_1(0)$	$-\psi_1'(0)$
0	0	0.999 (1)	0.729 (0.725)
	0.1	0.999 (1)	0.785 (0.751)
	0.2	0.999 (1)	0.851 (0.776)
	0.3	0.999 (1)	0.932 (0.801)
0.1	0	0.941	0.687
	0.1	0.937	0.733
	0.2	0.933	0.787
	0.3	0.928	0.848
1	0	0.617 (0.633)	0.451 (0.431)
	0.1	0.603 (0.627)	0.460 (0.438)
	0.2	0.596 (0.622)	0.476 (0.444)
	0.3	0.583 (0.616)	0.487 (0.450)
10	0	0.138	0.101
	0.1	0.137	0.101
	0.2	0.136	0.101
	0.3	0.135	0.101

$$\phi_1^{(k+1)}(0) = -\theta_3\psi_1'^{(k)}(0), \quad \xi_1 = 0$$

$$\phi_1'^{(k+1)}(0) = 2\theta_1\frac{\varepsilon_2}{\varepsilon_1}\phi_2'^{(k)}(0), \quad \xi_1 = \xi_2 = 0$$

$$\psi_1^{(k+1)}(0) = 1-\psi_2^{(k)}(0), \quad \xi_1 = \xi_2 = 0$$

$$\phi_1'^{(k+1)}(\infty) = 2\varepsilon_1^{-1}, \quad \xi_1 \to \infty$$

$$\psi_1^{(k+1)}(\infty) = 0, \quad \xi_1 \to \infty \quad (5)$$

where $\psi_1'^{(0)}(0)$, $\phi_2'^{(0)}(0)$ and $\psi_2^{(0)}(0)$ are prescribed initial guesses

$$\phi_2'''^{(k+1)} + 2\varepsilon_2^{-1}\phi_2^{(k+1)}\phi_2''^{(k+1)} = 0, \quad \xi_2 > 0$$

$$\psi_2''^{(k+1)} + 2\varepsilon_2\phi_2^{(k+1)}\psi_2'^{(k+1)} = 0, \quad \xi_2 > 0 \quad (6)$$

$$\phi_2^{(k+1)}(0) = \theta_4\psi_2'^{(k)}(0), \quad \xi_2 = 0$$

$$\phi_2''^{(k+1)}(0) = -\tfrac{1}{2}\theta_2\left(\frac{\varepsilon_1}{\varepsilon_2}\right)^2\phi_1''^{(k+1)}(0), \quad \xi_2 = \xi_1 = 0$$

$$\psi_2'^{(k+1)}(0) = \frac{\chi}{\varepsilon_0}\psi_1'^{(k+1)}(0), \quad \xi_2 = \xi_1 = 0$$

$$\phi_2'^{(k+1)}(\infty) = \varepsilon_2^{-1}, \quad \xi_2 \to \infty$$

$$\psi_2^{(k+1)}(\infty) = 0, \quad \xi_2 \to \infty \quad (7)$$

where $\psi_2'^{(0)}(0)$ is a prescribed initial guess.

For $\chi/\varepsilon_0 \geqslant 1$ the first three equations of equations (5) and (7) are replaced

$$\phi_1^{(k+1)}(0) = -\theta_3\psi_1'^{(k)}(0), \quad \xi_1 = 0$$

$$\phi_1'^{(k+1)}(0) = 2\theta_1\frac{\varepsilon_2}{\varepsilon_1}\phi_2'^{(k)}(0), \quad \xi_1 = \xi_2 = 0$$

$$\psi_1'^{(k+1)}(0) = \left(\frac{\chi}{\varepsilon_0}\right)^{-1}\psi_2'^{(k)}(0), \quad \xi_1 = \xi_2 = 0$$

$$\phi_2^{(k+1)}(0) = \theta_4\psi_2'^{(k)}(0), \quad \xi_2 = 0 \quad (8)$$

$$\phi_2''^{(k+1)}(0) = -\tfrac{1}{2}\theta_2\left(\frac{\varepsilon_1}{\varepsilon_2}\right)^2\phi_1''^{(k+1)}(0), \quad \xi_2 = \xi_1 = 0$$

$$\psi_2^{(k+1)}(0) = 1-\psi_1^{(k+1)}(0), \quad \xi_2 = \xi_1 = 0$$

$$k = 0, 1, 2, \ldots \quad (9)$$

where $\psi_1'^{(0)}(0)$, $\phi_2'^{(0)}(0)$ and $\psi_2'^{(0)}(0)$ are prescribed initial guesses.

The iteration loop parameter k takes values $0, 1, 2, \ldots, n$.

When $k = n$ there are two possibilities.

(a) $n \leqslant n_{\max}$.

The iterative process has been convergent in the sense that

$$\|y^{(n)} - y^{(n-1)}\| < \delta, \quad \|y\| \leqslant 1$$

$$\left|1 - \frac{\|y^{(n-1)}\|}{\|y^{(n)}\|}\right| < \delta, \quad \|y\| > 1 \quad (10)$$

where $\|\cdot\|$ is the Euclidean vector norm; $(\cdot)'$ denotes differentiation in the independent variable, ξ_1 or ξ_2, respectively; δ is the prescribed accuracy (usually an

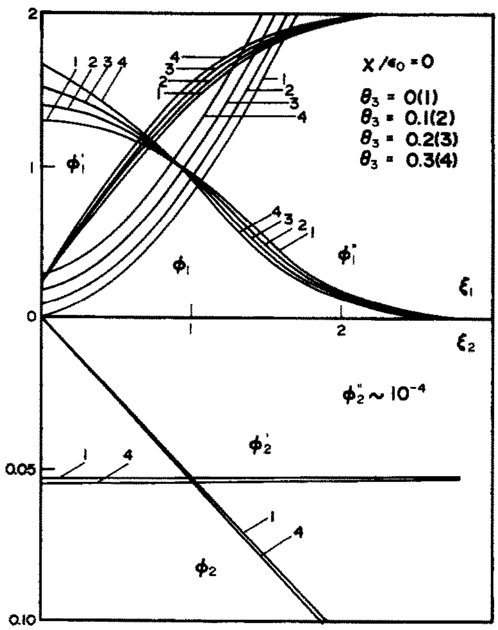

FIG. 1.

order of magnitude less than the accuracy of the solution of the corresponding boundary value problem), the vector y is defined as

$$y^{T} = \{\phi_1(0), \phi_1'(0), \phi_1''(0), \psi_1(0), \psi_1'(0), \phi_2(0), \phi_2'(0), \phi_2''(0), \psi_2(0), \psi_2'(0)\} \quad (11)$$

and n_{max} is the prescribed maximum admissible number of iterations.

(b) $n = n_{max}+1$ and the convergence criterion, equations (10) have not been satisfied.

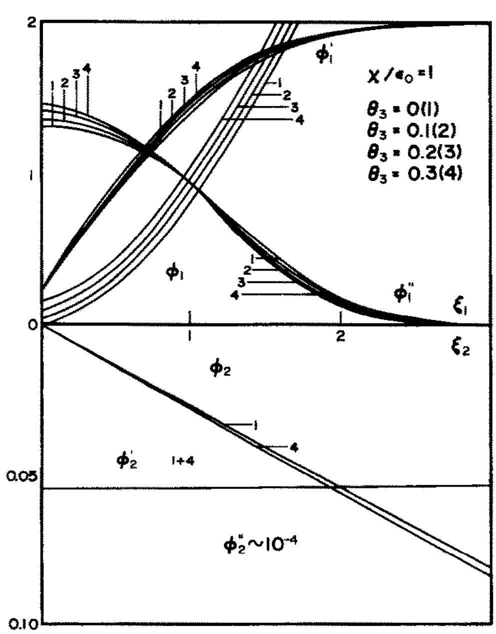

FIG. 2.

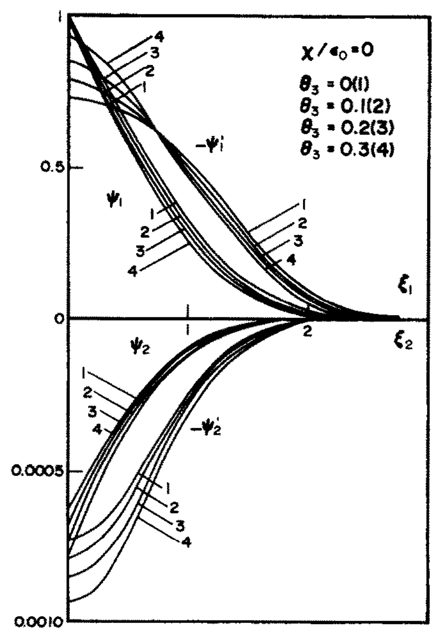

FIG. 3.

All quantities not explained in the text are listed in the Nomenclature of ref. [1]. The prescribed initial guesses mentioned in the above are taken as the values of the corresponding quantities assuming that non-linear effects are absent [3].

DISCUSSION OF THE NUMERICAL RESULTS

The iterative procedure described in the previous section was programmed in ANSI FORTRAN and numerical simulation was performed on an IBM

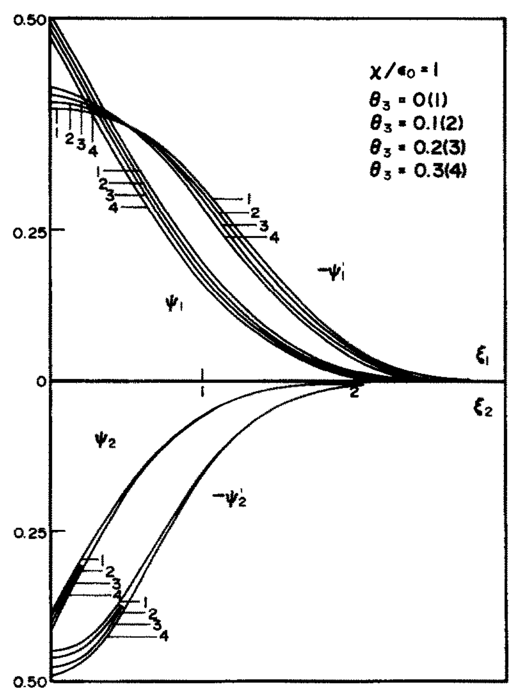

FIG. 4.

360/370 computer in OS environment. In all calculations to be described the following parameters were used: $\varepsilon_1 = 1$, $\varepsilon_2 = 20$, $\theta_1 = 0.1$, $\theta_2 = 0.152$, $\theta_4 = 0$, $\delta = 10^{-3}$, $n_{max} = 25$, $\chi/\varepsilon_0 = 10^{-3}, 0.1, 1, 10$, $\theta_3 = 0, 0.1, 0.2, 0.3$. Representative results for the calculated initial conditions (the vector as defined from equation (11)) are given in Tables 1 and 2. The calculated functions are shown on Figs. 1–4 and discussed in what follows. For fixed initial guesses [3] the rate of convergence varied with the values of χ/ε_0 and θ_3 being poor for θ_3 large and $\chi/\varepsilon_0 = 1$ $(n = 17)$ and very fast for $\theta_3 = 0$ and $\chi/\varepsilon_0 = 1$ $(n = 2)$—the initial guesses for this case were taken from ref. [3]. One iteration usually took about 5–6 min CPU time and comprises the successive integration of equations (4) and (5) or (8), and equations (6) and (7) or (9). For the gas (the first five components of y) the computational infinity was roughly six units in the dimensionless independent variable, while for the liquid (the last five components of y) it was in the range of 20–40 units.

THE VELOCITY DISTRIBUTIONS

The velocity distributions in the diffusion boundary layers are determined by the functions $\phi_1'(\xi_1)$ and $\phi_2'(\xi_2)$ (Figs. 1 and 2), for different values of χ/ε_0 and θ_3. These figures show the influence of the mass transfer on the hydrodynamics of the flow and, in particular, on the velocity component, normal to the phase interface and determined by the values of $\phi_1(0)$ and $\phi_2(0)$ (Table 1). In this table one can also find values for $\phi_1'(0)$ and $\phi_1''(0)$ calculated according to the previous section. In parentheses we have given the values of the same quantities as calculated by means of the asymptotic theory [1].

THE CONCENTRATION DISTRIBUTIONS

The concentration distributions $\psi_1(\xi_1)$ and $\psi_2(\xi_2)$ are shown on Figs. 3 and 4 for the corresponding values of χ/ε_0 and θ_3. From these figures one can see the non-linear effects in the gas and their influence on the mass transfer in the liquid. The corresponding values of $\psi_1(0)$ and $\psi_1'(0)$ as calculated according to the previous section are summarized in Table 2. Again, in parentheses we have listed the values of the same quantities calculated through the asymptotic theory [1].

In ref. [1] it was shown that the interphase mass transfer and the mass transfer in the separate phases are determined in a unique manner by the dimensionless diffusive fluxes $\psi_1'(0)$ and $\psi_2'(0)$ at the phase interface. Numerical data for these quantities can also be found in Table 2.

CONCLUSIONS

The numerical results obtained indicate that the non-linear effects in the gas phase are most pronounced for highly soluble gases $(\chi/\varepsilon_0 \to 0)$. When the solubility of the gas is moderate $(\chi/\varepsilon_0 \sim 1)$ the non-linear effects are still significant, but when the solubility of the gas decreases $(\chi/\varepsilon_0 \gg 1)$ they can be neglected.

The non-linear effects in the liquid are the result of the non-linear mass transfer in the gas. They are negligible in respect to the hydrodynamics. Mass transfer in the liquid depends most strongly on the non-linear effects in the gas for moderately soluble gases $(\chi/\varepsilon_0 \sim 1)$. For highly soluble gases $(\chi/\varepsilon_0 \to 0)$ and weakly soluble ones $(\chi/\varepsilon_0 > 10^2)$ it is negligible because in the former case the mass transfer is limited only by the gas, while in the latter one, the non-linear effects can be neglected.

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TRANSFERT DE MASSE NON LINEAIRE DANS DES COUCHES LIMITES— 2. ETUDE NUMERIQUE

Résumé—La solution numérique d'une classe de problèmes pour le transfert de masse non linéaire dans des couches limites laminaire de diffusion, d'un système gaz–liquide, est obtenue en utilisant une procédure numériquement stable pour l'intégration des systèmes d'équations différentielles. On considère l'influence de la solubilité du gaz et des effets non linéaires dans le gaz sur l'hydrodynamique et le transfert de masse. On présente aussi des résultats numériques.

NICHTLINEARER MASSENTRANSPORT IN GRENZSCHICHTEN—2. NUMERISCHE UNTERSUCHUNG

Zusammenfassung—Es wird die numerische Lösung einer Klasse von Problemen des nichtlinearen Massentransports in laminaren Diffusionsgrenzschichten für Gas–Flüssigkeits-Systeme ermittelt. Zur numerischen Integration der asymptotischen Grenzwertprobleme bei Systemen gewöhnlicher Differentialgleichungen wird ein numerisch stabiles Verfahren vom Erhaltungstyp verwendet. Der Einfluß der Gaslöslichkeit und nichtlinearer Effekte im Gas auf die Hydrodynamik und den Massentransport wurden untersucht. Es werden numerische Ergebnisse vorgestellt.

НЕЛИНЕЙНЫЙ МАССООБМЕН В ПОГРАНИЧНЫХ СЛОЯХ—2. ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ

Аннотация—Используя устойчивый, непрерывного типа метод численного интегрирования асимптотических граничных задач для систем обыкновенных дифференциальных уравнений, называемый методом пристрелки, получено численное решение класса задач нелинейного массопереноса в ламинарном диффузионном пограничном слое для систем 'газ–жидкость'. Изучено влияние растворимости газа и нелинейных эффектов в газе на гидродинамику и массоперенос. Представлены численные результаты.