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Some mathematical results for impurity redistribution during the growth of a layer on a substrate

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Résumé. — Ce travail présente une série de résultats pour la redistribution par diffusion d’une impureté initialement distribuée de façon homogène dans un substrat, au cours de la croissance d’une couche sur ce substrat. Il présente également des résultats sur la diffusion, au cours du même processus de croissance, d’une impureté provenant d’une phase extérieure. Dans les deux cas on étudie le cas d’une couche dont la nature est différente de celle du substrat.

Outre les résultats analytiques obtenus, un intérêt de ce travail peut résider dans la méthode mathématique utilisée pour les établir, telle qu’elle est exposée en appendice (applicable dans les cas où la vitesse de croissance de la couche est une constante).

Abstract. — This work presents a series of results for the redistribution by diffusion of an impurity initially distributed homogeneously in a substrate during the growth of a layer on this substrate. It also gives results concerning the diffusion during the same growth process of an impurity coming from an exterior phase. In both cases the nature of the layer is different from that of the substrate.

In addition to the obtained analytical results, the mathematical method used to obtain them is also of interest. This is described in the appendix (case when the growth rate of the layer is a constant).

1. Introduction. — The problem of the diffusional distribution of impurities during the growth of a layer on a substrate is of great practical importance for metallurgists, particularly in the case of semiconducting compounds whose electronic properties depend strongly on the presence and shape of the impurities concentration profiles.

Some results on this subject have previously been established in the case where the layer is of the same nature as the substrate and in presence (or not) of an evaporation flux at the surface of the growing layer (see for instance ref. [1]).

In this study we want to extend these types of results to the case where the layer is of a different nature from the substrate regarding either the diffusion properties (diffusion coefficients) or the solubility limit of the impurity (segregation coefficient at the interface) or both.

The paper is devoted to the case of the redistribution during the growth of an impurity initially homogeneously distributed in the substrate.

In the limiting case where the diffusive and segregative properties of the layer become the same as those of the substrate, our present treatment reproduces the classical results.

Throughout this paper we have always made the following assumptions:

— Fick’s laws for diffusion are applicable.
— The diffusion coefficients are considered to be constant (and particularly to be concentration independent).
— The rate of growth of the layer, \( V \), is considered to be constant.

We have used the tables of Laplace and inverse Laplace transforms quoted in references [2] and [3], with some other results that we have derived from them.

Notations

\[ V : \text{rate of growth of the layer.} \]
\[ D_1 : \text{diffusion coefficient in the substrate} \]
\[ D_2 : \text{diffusion coefficient in the layer} \]

whatever the nature of the impurity.

\[ K : \text{segregation coefficient of an impurity between the layer and the substrate.} \]
\( x \) : distance from the origin 0 which is at the initial surface of the substrate, measured positively in the direction of the layer surface.

\( t \) : time.

\( p \) : Laplace's time conjugated variable.

\( C_1 \) : relative concentration in the substrate of the impurity initially present in the substrate.

\( C_2 \) : relative concentration in the layer of this impurity.

\( C_1' \) : relative concentration in the substrate of the impurity coming from the outer phase.

\( C_2' \) : relative concentration in the layer of this impurity.

\( C_{2s} \) : constant surface concentration of this impurity.

\( Y(y) \) : Heaviside's distribution (\( Y(y) = 1 \) for \( y > 0 \), \( Y(y) = 0 \) for \( y < 0 \)).

\( \sigma = 1 - K \frac{D_1}{\sqrt{D_2}} \)

\( \rho = 1 + K \frac{D_1}{\sqrt{D_2}} \).

The configuration is represented in figure 1.

Fig. 1. — Schematic representation of the system.

2. Redistribution. — In order to be rigorous in the treatment of this type of problem we formalized it in the following way:

a) To take into account the discontinuity due to the surface of the layer (considered as impermeable for the impurity coming from the inside) and the discontinuity due to the separation between the layer and the substrate where the diffusive properties are different, we choose a discontinuous diffusion coefficient:

\[
D = D_1 Y(-x) + D_2 [Y(Vt - x) - Y(-x)].
\]  

(1)

b) To deal with «good» convergent functions and in order to eliminate the presence of the disturbing and useless \( \delta \) distribution, we choose as a fundamental function, the function:

\[
\Gamma(x, t) = \int_{-\infty}^{\infty} [1 - C_1(X, t)] dX
\]

(2)

which offers the advantage of being always convergent (because for \( x \to -\infty \), \( C_1 \to 1 \) and \( \Gamma \to 0 \)). For \( x \leq 0 \), it represents the loss of matter (impurity) initially present in this region, due to the diffusion.

Fick's basic equation is:

\[
\frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial C_1}{\partial x} \right)
\]

(3)

with the initial condition:

\[
C_1(x, t = 0) = Y(-x)
\]

(4a)

and the boundary conditions:

\[
C_1(0^-, t) = KC_2(0^+, t)
\]

(4b)

\[
D_1 \left( \frac{\partial C_1}{\partial x} \right)_{x=0^-} = D_2 \left( \frac{\partial C_2}{\partial x} \right)_{x=0^+}
\]

(4c)

\[
\int_{-\infty}^{0} (1 - C_1) \, dx = \int_{0}^{\nu t} C_2 \, dx
\]

(4d)

0\(^-\) et 0\(^+\) indicate the value of \( x \) at 0 from negative and positive side respectively. (4b) is the segregation condition. (4c) is the flux conservation condition at the interface between the layer and the substrate and (4d) is the impurity total quantity conservation condition (impermeable surface of the layer).

In terms of function (2), all these equations take the corresponding forms:

\[
\frac{\partial \Gamma}{\partial t} = D \frac{\partial^2 \Gamma}{\partial x^2}.
\]

(5)

With the initial condition:

\[
\Gamma(x, t = 0) = xY(x)
\]

(6a)

\[
1 - \left( \frac{\partial \Gamma}{\partial x} \right)_{0^-} = K \left[ 1 - \left( \frac{\partial \Gamma}{\partial x} \right)_{0^+} \right]
\]

(6b)

\[
\Gamma(0^-, t) = \Gamma(0^+, t)
\]

(6c)

\[
\Gamma(Vt, t) = Vt
\]

(6d)

Fig. 2. — Theoretical results from eq. (7).
To obtain the solution we have to distinguish between the two regions: $x < 0$ (corresponding concentration $C_1$) and $x > 0$ ($C_2$).

The calculation is quite tedious because of the time-dependent boundary condition; it is given in the appendix.

The result is:

$$C_1 = 1 - \frac{1}{\rho} \left\{ \text{erfc} \left( \frac{-x}{2\sqrt{D_1}t} \right) \right\} - \left( 1 - \frac{\sigma}{\rho} \right) \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \left\{ \text{erfc} \left( \frac{-k(1+V)x}{\sqrt{D_1} D_2} \right) \times \right.$$  

$$\times \exp \left( \frac{(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( \frac{-x}{2\sqrt{D_1} t} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \times \left( 1 - \frac{(k+1) V x}{\sqrt{D_2} D_2} + \frac{2(k+1)^2 V^2 t}{D_2} \right)$$

$$- 2(k+1) V \sqrt{t} \exp \left( -\frac{x^2}{4 D_1 t} \right) \right\}$$  

$$C_2 = \frac{1}{\rho} \sqrt{\frac{D_1}{D_2}} \left\{ \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} \right) \right\} + \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \left\{ \frac{\sigma}{\rho} - 2 V(k+1) \frac{t}{\pi D_2} \exp \left( -\frac{x^2}{4 D_2 t} \right) + \right.$$  

$$\exp \left( \frac{(k+1) V x}{D_2} + \frac{(k+1)^2 V^2 t}{D_2} \right) \left( 1 + \frac{(k+1) V x}{D_2} + \frac{2(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$+ \left( \exp \left( -\frac{(k+1) V x}{D_2} + \frac{(k+1)^2 V^2 t}{D_2} \right) \left( 1 - \frac{(k+1) V x}{D_2} + \frac{2(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2} t} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$- 2 V(k+1) \sqrt{t} \exp \left( -\frac{x^2}{4 D_2 t} \right) \right\}$$  

It is easy to verify that for the limit $D_1 = D_2 = D$, $K = 1$, then $\sigma = 0$, $\rho = 2$ and we recover the simple result of reference [1], in the absence of an evaporation flux at the surface.

An illustration of this result is given in figure 2 which represents equation (7) calculated numerically for various values of the parameters.

From a numerical point of view some practical problems arise because of the very great values of exponential factors and the very low value of erfc for high values of $k$. In these cases it is convenient to take the asymptotic development of the erfc, for instance for $k \geq N$ (depending on the values of the various parameters), we have to add to the expression (7) for $k < N$, the approximate expression (for $k \geq N$) (denoted with the index (as) for asymptotic)

$$C_{1\text{as}} = \frac{1}{\rho} \left( 1 - \frac{\sigma}{\rho} \right) \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \frac{1}{\sqrt{\pi}} \exp \left( -\frac{x^2}{4 D_1 t} \right)$$

$$\sqrt{\frac{D_2}{D_1}} \frac{x}{\sqrt{D_1}} \frac{(k+1) V \sqrt{t}}{\sqrt{2 D_1 t}} + \frac{x}{\sqrt{2 D_1 t}}.$$  

$$C_{2\text{as}} = \frac{1}{\rho} \sqrt{\frac{D_1}{D_2}} \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \exp \left( -\frac{x^2}{4 D_2 t} \right) \frac{\sigma}{\rho} \frac{x}{2\sqrt{D_2 t}} + \frac{\sqrt{D_2}}{(k+1) V \sqrt{t} - \frac{x}{\sqrt{2 D_2 t}}}. (7)$$

3. Diffusion from the outside. — The same type of analysis and calculation leads to the result:

$$C_1' = \frac{C_{2\text{as}}}{2} \sqrt{\frac{D_2}{D_1}} \left( 1 - \frac{\sigma}{\rho} \right) \sum_{k=0}^{\infty} \left( - \frac{\sigma}{\rho} \right)^k \left[ \exp \left( -\frac{k V x}{\sqrt{D_1 D_2}} + \frac{k^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_1 t}} + \frac{k V \sqrt{t}}{\sqrt{D_2}} \right) + \right.$$  

$$\exp \left( -\frac{(k+1) V x}{\sqrt{D_1 D_2}} + \frac{(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2 t}} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$+ \left( \exp \left( -\frac{(k+1) V x}{D_2} + \frac{(k+1)^2 V^2 t}{D_2} \right) \left( 1 - \frac{(k+1) V x}{D_2} + \frac{2(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2 t}} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$- 2 V(k+1) \sqrt{t} \exp \left( -\frac{x^2}{4 D_2 t} \right) \right\}$$  

$$C_2' = \frac{C_{2\text{as}}}{2} \left\{ \sum_{k=0}^{\infty} \left( - \frac{\sigma}{\rho} \right)^k \left[ \exp \left( -\frac{k V x}{D_2} + \frac{k^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2 t}} + \frac{k V \sqrt{t}}{\sqrt{D_2}} \right) + \right.$$  

$$\exp \left( -\frac{(k+1) V x}{D_2} + \frac{(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2 t}} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$+ \left( \exp \left( -\frac{(k+1) V x}{D_2} + \frac{(k+1)^2 V^2 t}{D_2} \right) \left( 1 - \frac{(k+1) V x}{D_2} + \frac{2(k+1)^2 V^2 t}{D_2} \right) \text{erfc} \left( -\frac{x}{2\sqrt{D_2 t}} + \frac{(k+1) V \sqrt{t}}{\sqrt{D_2}} \right) \right.$$  

$$- 2 V(k+1) \sqrt{t} \exp \left( -\frac{x^2}{4 D_2 t} \right) \right\}.$$  

(8)
The concentration at the surface of the layer has been taken to be constant \( (C_0) \).

The same remarks as above are true for large values of \( k \). In this case the corresponding terms for \( k \geq N \) take the form:

\[
C_{1_{as}} = \frac{C_{2s}}{2} \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \left[ \exp \left( \frac{k V x}{D_2} + \frac{k^2 V^2 t}{D_2} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} + \frac{k V \sqrt{t}}{D_2} \right) + \right.
\]
\[
+ \exp \left( \frac{(k + 1) V x}{D_2} + \frac{(k + 1)^2 V^2 t}{D_2} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} + \frac{(k + 1) V \sqrt{t}}{D_2} \right) \right] .
\]

The concentration at the surface of the layer has been taken to be constant \( (C_0) \).

The same remarks as above are true for large values of \( k \). In this case the corresponding terms for \( k \geq N \) take the form:

\[
C_{2_{as}} = \frac{C_{2s}}{2} \sum_{k=0}^{\infty} \left( \frac{\sigma}{\rho} \right)^k \left[ \exp \left( \frac{x^2}{4 D_2 t} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} + \frac{k V \sqrt{t}}{D_2} \right) + \right.
\]
\[
+ \exp \left( \frac{(k + 1) V x}{D_2} + \frac{(k + 1)^2 V^2 t}{D_2} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} + \frac{(k + 1) V \sqrt{t}}{D_2} \right) \right] .
\]

4. **Solubility limit at the interface.** — In the case where no proportional segregation occurs at the interface, but only a solubility limit condition is imposed on the impurity concentration in the layer (solubility limit defined as \( C_0 \) in the layer), then the condition at the interface takes the form:

\[
1 - \left( \frac{\partial C}{\partial x} \right)_0 = C_0 (\leq C_1 (x = 0^-)).
\]

The same type of procedure as the preceding one (cf. appendix) leads to the following result:

\[
C_1 = 1 - C_2^o \sqrt{\frac{D_2}{D_1}} \text{erfc} \left( \frac{x}{2\sqrt{D_1} t} \right) - 2 C_2^o \sqrt{\frac{D_2}{D_1}} \sum_{k=0}^{\infty} (-1)^k \left[ - \frac{2(k + 1) V}{\sqrt{D_1} D_2} \exp \left( \frac{x^2}{4 D_1 t} \right) + \right.
\]
\[
+ \left( 1 - (k + 1) \frac{V}{\sqrt{D_1} D_2} + \frac{2(k + 1)^2 V^2}{D_2} \right) \text{erfc} \left( \frac{x}{2\sqrt{D_1} t} + \frac{(k + 1) V \sqrt{t}}{D_2} \right) \right] \times
\]
\[
C_2 = C_2^o \text{erfc} \left( \frac{x}{2\sqrt{D_2} t} \right) + C_2^o \sum_{k=0}^{\infty} (-1)^k \left[ \left( 1 + (k + 1) \frac{V}{\sqrt{D_1} D_2} + \frac{2(k + 1)^2 V^2}{D_2} \right) \times
\]
\[
\times \exp \left( \frac{(k + 1) V x + (k + 1)^2 V^2 t}{D_2} \right) \right] \times
\]
\[
\text{erfc} \left( \frac{x}{2\sqrt{D_1} t} + \frac{(k + 1) V \sqrt{t}}{D_2} \right) - \left( 1 - (k + 1) \frac{V}{\sqrt{D_1} D_2} + \frac{2(k + 1)^2 V^2}{D_2} \right) \right] \times
\]
\[
\text{erfc} \left( \frac{x}{2\sqrt{D_1} t} + \frac{(k + 1) V \sqrt{t}}{D_2} \right) \right].
\]

In the case of an impurity coming from the outer phase during the growth and submitted to the same type of solubility limit at the interface, but this time for the substrate, the condition \( C(|0^-|) = C_1^s \) leads of course to the well known \( \text{erfc} \) behaviour in the substrate:

\[
C' = C_1^s \text{erfc} \left( \frac{x}{2\sqrt{D_1} t} \right).
\]
The asymptotic parts for $k > N$ in expression (9) are, respectively:

$$C_{1as} = -2 C_2^0 \sqrt{\frac{D_2}{D_1}} \sum_{k=N}^{\infty} (-1)^k \frac{\exp\left(-\frac{x^2}{4 D_1 t}\right)}{\sqrt{\pi} \left(\frac{x}{2 \sqrt{D_1 t}} + \frac{(k + 1) V \sqrt{t}}{\sqrt{D_2}}\right)}$$

$$C_{2as} = C_2^0 \sum_{k=N}^{\infty} (-1)^k \frac{x}{\sqrt{\pi D_2 t}} \frac{\exp\left(-\frac{x^2}{4 D_2 t}\right)}{(k + 1)^2 V^2 t - \frac{x^2}{D_2} - \frac{4 D_2 t}{D_2}}$$

(9')

5. Conclusion.— It has been possible to calculate exactly, in a tractable mathematical form, the shapes of the concentration profiles in the cases of diffusion or redistribution of impurities during the growth of a layer on a substrate. Various situations have been investigated such as segregation at the interface and different diffusion coefficients in the substrate and in the layer.

These results are directly applicable in actual situations and some approximations have been given to facilitate the calculation techniques themselves.

Appendix.— Calculation for the conditions of § 1.— For $x < 0$ we designate the function $\Gamma$ as $\Gamma_1$ and for $x > 0$ as $\Gamma_2$. The starting equations are:

$$\frac{\partial \Gamma_1}{\partial t} = D_1 \frac{\partial^2 \Gamma_1}{\partial x^2} \quad \text{(A.1)}$$

$$\frac{\partial \Gamma_2}{\partial t} = D_2 \frac{\partial^2 \Gamma_2}{\partial x^2} \quad \text{(A.1')}

Taking the Laplace transforms of both equations with the specified initial conditions leads to:

$$p \Gamma_{1p} = D_1 \frac{\partial^2 \Gamma_{1p}}{\partial x^2} \quad \text{(A.2)}$$

$$p \Gamma_{2p} - x = D_2 \frac{\partial^2 \Gamma_{2p}}{\partial x^2} \quad \text{(A.2')}

The solutions of these equations are:

$$\Gamma_{1p} = A(p) \exp\left(\frac{x}{\sqrt{D_1}} \sqrt{p}\right) + B(p) \exp\left(-\frac{x}{\sqrt{D_1}} \sqrt{p}\right) \quad \text{(A.3)}$$

$$\Gamma_{2p} = F(p) \exp\left(\frac{x}{\sqrt{D_2}} \sqrt{p}\right) + G(p) \exp\left(-\frac{x}{\sqrt{D_2}} \sqrt{p}\right) \quad \text{(A.3')}

As $r \to 0$ when $x \to -\infty$, we must put $B(p) = 0$ in equation (A.3).

The remaining coefficients $A(p), F(p), G(p)$ have to be determined by the various boundary-conditions.

From $\Gamma_{2p}(0) = \Gamma_{1p}(0)$, we obtain:

$$A(p) = F(p) + G(p) \quad \text{(A.4)}$$

From $1 - \left(\frac{\partial \Gamma_1}{\partial x}\right)_0 = K \left(1 - \left(\frac{\partial \Gamma_2}{\partial x}\right)_0\right)$ we obtain

$$A(p) = \sqrt{\frac{D_1}{p \sqrt{p}}} + K \sqrt{\frac{D_1}{D_2}} [F(p) - G(p)] \quad \text{(A.5)}$$

Eliminating $A(p)$ between (A.4) and (A.5) leads to:

$$\sigma F(p) + \rho G(p) = \sqrt{\frac{D_2}{p \sqrt{p}}} \quad \text{(A.6)}$$
The last condition is to be written at \( x = V t(\sqrt{D_2}, t) = V t \), but to avoid mixing the time variable \( t \) with its Laplace conjugate \( p \), we prefer to write (\( \mathcal{C}_i \) meaning the inverse Laplace transform operator):

\[
\mathcal{C}_i \left[ F(p) \exp \left( \frac{x}{\sqrt{D_2}} \sqrt{p} \right) + G(p) \exp \left( - \frac{x}{\sqrt{D_2}} \sqrt{p} \right) \right]_{x=V t} = 0 \quad (A.7)
\]

with

\[
\mathcal{C}_i = (2 \pi i)^{-1} \int_{c-i\infty}^{c+i\infty} e^{\pi p} \, dp.
\]

Explicitly:

\[
(2 \pi i)^{-1} \int_{c-i\infty}^{c+i\infty} dp \left[ F(p') \exp \left( \frac{V t}{\sqrt{D_2}} \sqrt{p'} \right) e^{\pi p'} + G(p') \exp \left( - \frac{V t}{\sqrt{D_2}} \sqrt{p'} \right) e^{\pi p'} \right] = 0.
\]

In the factor of \( F(p') \) we perform the transformation \( p' + \sqrt{p'} \frac{V}{\sqrt{D_2}} \rightarrow p \) and \( p' - \frac{V}{\sqrt{D_2}} \sqrt{p'} \rightarrow p \) in the factor of \( G(p') \) (with the corresponding transformation for the differential). We obtain then, dropping the inessential factor \( (2 \pi i)^{-1} \):

\[
\int_{c-i\infty}^{c+i\infty} dp \left\{ F \left[ \left( \sqrt{p} + \frac{V^2}{4 D_2} - \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( 1 - \frac{V}{2 \sqrt{D_2}} \sqrt{p + \frac{V^2}{4 D_2}} \right) e^{\pi p} + \right.
\]

\[
\left. + G \left[ \left( \sqrt{p} + \frac{V^2}{4 D_2} + \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( 1 + \frac{V}{2 \sqrt{D_2}} \sqrt{p + \frac{V^2}{4 D_2}} \right) e^{\pi p} \right\} = 0.
\]

With the further transformation of \( p \rightarrow p - \frac{V^2}{4 D_2} \), and dropping the new factor \( e^{\pi \frac{V^2}{4 D_2}} \), we finally obtain the relation:

\[
F \left[ \left( \sqrt{p} - \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( \sqrt{p} - \frac{V}{2 \sqrt{D_2}} \right) + G \left[ \left( \sqrt{p} + \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( \sqrt{p} + \frac{V}{2 \sqrt{D_2}} \right) = 0, \quad (A.8)
\]

which can also be written (putting \( \frac{\sqrt{p} + V}{2 \sqrt{D_2}} \rightarrow \sqrt{p} \))

\[
F \left[ \left( \sqrt{p} - \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( \sqrt{p} - \frac{V}{2 \sqrt{D_2}} \right) + G(p) \sqrt{p} = 0. \quad (A.9)
\]

Bringing (A.9) into (A.6), we obtain for \( F \), the functional relation:

\[
\sigma F(p) - \rho F \left[ \left( \sqrt{p} - \frac{V}{2 \sqrt{D_2}} \right)^2 \right] \left( 1 - \frac{V}{\sqrt{p D_2}} \right) = \frac{\sqrt{D_1} p^2}{\sqrt{\rho p}}. \quad (A.10)
\]

Introducing for convenience the dimensionless variable \( \varphi \), such that

\[
\sqrt{\varphi} = \frac{\sqrt{D_2} p}{V}
\]

we have:

\[
\sigma \sqrt{\varphi} F[\sqrt{\varphi}] - \rho F[\sqrt{\varphi} - 1] (\sqrt{\varphi} - 1) = \frac{D_2 \sqrt{D_1} D_2}{\rho V^3}
\]

which can functionally be written:

\[
\sigma \sqrt{\varphi} E[\sqrt{\varphi}] - \rho E[\sqrt{\varphi} - 1] (\sqrt{\varphi} - 1) = \frac{D_2 \sqrt{D_1} D_2}{\rho V^3}. \quad (A.11)
\]
Performing the transformation $\sqrt{\varphi} \to \varphi'$, (A.11) becomes:

$$\sigma \varphi' E(\varphi') - \rho (\varphi' - 1) E(\varphi' - 1) = \frac{D_2 \sqrt{D_1 D_2}}{\sigma^2 V^3}.$$

(A.12)

To solve (A.12) we remark that it is the Laplace transform of a differential equation, namely (with $f(0) = 0$; $E(\varphi') \equiv f(y)$)

$$\sigma \frac{\partial f}{\partial y} - \rho \ e^y \frac{\partial f}{\partial y} = \frac{D_1 D_2}{V^3} D_2 y$$

$$\frac{\partial f}{\partial y} = \frac{D_2 \sqrt{D_1 D_2}}{V^3} \frac{y}{\sigma - \rho \ e^y}.$$

(A.13)

We can then write ($\mathcal{L}$ denoting the Laplace transform operator):

$$E(\varphi') = \frac{D_2 \sqrt{D_1 D_2}}{V^3} \mathcal{L} \int_0^\varphi \frac{y \ dy}{\sigma - \rho \ e^y}$$

$$= \frac{D_2 \sqrt{D_1 D_2}}{V^3} \left[ \frac{y}{\varphi'} \mathcal{L} \int_0^\varphi \frac{1}{\sigma - \rho \ e^y} \right]$$

$$= - \frac{D_2 \sqrt{D_1 D_2}}{V^3} \rho \sum_{k=0}^{\infty} \frac{(\sigma/\rho)^k}{(\varphi' + 1 + k)^2} \left( \frac{\sigma}{\rho} \right) \text{ is always < 1}. $$

Returning to $\sqrt{\varphi} \equiv \varphi'$ and then to $\rho$, we have finally:

$$F(p) = - \frac{\sqrt{D_1}}{\rho} \frac{1}{\sqrt{p}} \sum_{k=0}^{\infty} \frac{(\sigma/\rho)^k}{\sqrt{p + (k + 1) V^3 / (D_2)}}.$$

(A.14)

With the result (A.14), $G(p)$ can easily be calculated from (A.6), and then $A(p)$ from (A.4). Putting these coefficients in the expressions (A.3), (A.3') leads to the results of §1.

To obtain the results of §2, the same method has been used.

Remark: During the course of the calculations, some remarkable equalities appeared depending on the method we used to evaluate them. Particularly, it has been possible to establish the following results for integrals:

$$\int_0^\infty (v - u) v^{-3/2} \exp\left[-\frac{1}{4} \left(v + \frac{u^2}{v}\right)\right] \ dv' = \int_0^\infty \ dx \left[ \int_0^\infty \ dy \ y^{-3/2} \exp\left[-\frac{1}{4} \left(y + \frac{u^2}{y}\right)\right] \right] =$$

$$= \frac{\sqrt{\pi}}{u} \exp\left[-\frac{u}{2}\right] \left( \left(v - u\right) \text{erfc}\left(\frac{u}{2\sqrt{v}} - \frac{\sqrt{v}}{2}\right) + \left(v + u\right) \text{erfc}\left(\frac{u}{2\sqrt{v}} + \frac{\sqrt{v}}{2}\right) \right) \equiv \sqrt{\pi} \left( \text{erf}\left(\frac{v}{2}\right) - \frac{v}{2}\right) g(v, u),$$

and, of course, by simple derivation:

$$\int_0^\infty \ dx \ x^{-3/2} \exp\left[-\frac{1}{4} \left(x + \frac{u^2}{x}\right)\right] = \frac{\sqrt{\pi}}{u} \exp\left[-\frac{u}{2}\right] \frac{\partial}{\partial \nu} g(v, u).$$

At our knowledge this integral has not previously been calculated.

References

