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A diffusion problem in a cylindrical tube

by

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1. Introduction.

In this note we consider the diffusion of a uniformly moving substance in a cylindrical tube, the cross-section of which is the sector $0 \leq r \leq a$, $\varphi_1 \leq \varphi \leq \varphi_2$ in polar coordinates (r, φ). The combined process of diffusion and convection may be described by the equation

$$(1.1) \qquad D \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) + \frac{D'}{r^2} \frac{\partial^2 c}{\partial \varphi^2} = v \frac{\partial c}{\partial z} ,$$

where $c\,(r, \varphi, z)$ is the concentration of the substance, where D and D' are coefficients of diffusion and v is the systematic velocity which is assumed to be constant.
In this equation the effect of axial diffusion has been neglected. Assuming that at the entrance of the tube $(z=0)$ the concentration is a given function of r only,

$$(1.2) \qquad c = c_0(r) \qquad \text{at} \qquad z=0 ,$$

it is easily seen that the concentration will not depend on φ so that there only remains the effect of the radial diffusion.
The other boundary conditions are

$$(1.3) \qquad c \quad \text{continuous} \quad \text{at } r=0 ,$$

$$(1.4) \qquad \frac{\partial c}{\partial r} = 0 \quad \text{at} \quad r=a ,$$

$$(1.5) \qquad \frac{\partial c}{\partial \varphi} = 0 \quad \text{at} \quad \varphi=\varphi_1 , \varphi=\varphi_2 .$$

The latter two conditions simply express the fact that there is no flow across the wall of the tube. The last condition is fulfilled automatically if c does not depend on φ .

With the assumption (1.2) it will be shown in section 2 that the concentration at an arbitrary point is given by a series, the first two terms of **which are given below**

$$(1.6) \quad c(r,z) = \frac{2}{a^2}\int_0^a r\, c_o(r)\, dr + \frac{2e^{p_1 z}}{a^2}\frac{J_o(\frac{r}{a}\beta_1)}{J_o^{\,2}(\beta_1)}\int_0^a r\, c_o(r) \cdot J_o(\frac{r}{a}\beta_1)\, dr + \dots,$$

where $p_1 = -(a^2 v)^{-1} D \beta_1^{\,2}$ and $\beta_1 = 3.8317$ is the first positive zero of $J_1(x)$.

The first term represents the stationary situation which would be obtained by ideal mixing of the substance at the entrance. The second term shows the effect of diffusion and convection for points not too close to the entrance.

In section 3 we consider the special case

$$(1.7) \qquad c_o(r) = \begin{cases} 0 & \text{for } 0 \leq r \leq r_o , \\ 1 & \text{"} \quad r_o \leq r \leq a , \end{cases}$$

so that the above given solution (1.6) may be simplified as

$$(1.8) \quad c(r,z) = \frac{a^2 - r_o^{\,r}}{a^2} - \frac{2r_o e^{p_1 z}}{a\beta_1} J_1(\frac{r_o}{a}\beta 1) \frac{J_o(\frac{r}{a}\beta_1)}{J_o^2(\beta_1)} + \dots$$

The values of $J_o(\frac{r}{a}\beta_1)$, $J_o(\beta_1)$ and $J_1(\frac{r_o}{a}\beta_1)$ may be found in tables ([3] and [4]). We point out that these solutions hold for any sectorial cross-section since the values of φ_1 and φ_2 do not occur in the final expressions.

In the appendix we shall derive some formulae which are used in the sections 2 and 3.

References.

The equation of heat transport, which is analogous to the diffusion equation is treated in [1] and [2] ,

[1] Carslaw and Jaeger — Conduction of heat in solids. Oxford, 2nd ed. (1959), ch. VII.

[2] J. Crank — The mathematics of diffusion. Oxford, Clarendon Press (1956) ch.s I,II,V,XI and XII.

Tables:

[3] Jahnke-Emde — Tables of functions with formulae and curves. English-German Dover edition (1945), pp 156-166 (4 decimals).

[4] Royal Soc.Math.Tables. Vol.7: Bessel functions Part III: Zeros and associated values, p.2 (7 decimals).

[5] H.B. Dwight — Tables of intergrals and other mathematical data. Macmillan Comp. (1955), pp. 176-182.

2. Solution of the diffusion equation.

In this section we derive a solution of the equation (1.1), assuming that the concentration c does not depend on φ . Then (1.5) is fulfilled automatically, furthermore $\frac{\partial^2 c}{\partial \varphi^2} \equiv 0$ so we have to solve the simpler equation

$$(2.1) \qquad D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) = v\,\frac{\partial c}{\partial z}$$

with the boundary conditions

(2.2) $\quad c$ continuous at $r=0$,

(2.3) $\quad \frac{\partial c}{\partial r} = 0$ at $r=a$.

Applying Laplace transformation with respect to z:

$$(2.4) \quad \bar{c} = \bar{c}(r,p) = \int_0^{\infty} \exp(-pz) \quad c(r,z) \, dz,$$

we get the ordinary differential equation

$$D\left(\frac{d^2\bar{c}}{dr^2} + \frac{1}{r} \frac{d\bar{c}}{dr}\right) = v\,(p\bar{c} - c_o(r)) ,$$

which will be written in the form

$$(2.5) \quad \frac{d^2\bar{c}}{dr^2} + \frac{1}{r} \frac{d\bar{c}}{dr} - \alpha^2\bar{c} = a(r) ,$$

where $\alpha^2 = pv\,D^{-1}$ and $a(r) = -vD^{-1}c_o(r)$. This equation is of the Bessel type; its general **solution consists of a particular** solution and an arbitrary linear combination of the modified Bessel functions $I_o(\alpha r)$ and $K_o(\alpha r)$.
Using the method of variation of the constants a particular solution of (2.5) will be sought in the form

$$\bar{c} = A(r) \; I_o(\alpha r) + B(r) \; K_o(\alpha r).$$

The standard technique of this method gives the two relations

$$\begin{cases} A' \; I_o(\alpha r) + B' \; K_o(\alpha r) = 0 , \\ A' \; I_o'(\alpha r) + B' \; K_o'(\alpha r) = \alpha^{-1}a(r). \end{cases}$$

Solving these equations for A' and B' and applying the well-known property

$$I_o(x) \; K_o'(x) - I_o'(x) \; K_o(x) = -x^{-1} ,$$

we obtain

$$\begin{cases} A' = r \;\; a(r) \;\; K_o(\alpha r) , \\ B' = -r \;\; a(r) \;\; I_o(\alpha r). \end{cases}$$

Since we only need a particular solution we may put

$$\begin{cases} A = -\dfrac{V}{D}\displaystyle\int_0^r \rho\, c_o(\rho) \; K_o\,(\alpha\rho)\, d\rho \,, \\[2ex] B = \dfrac{V}{D}\displaystyle\int_0^r \rho\, c_o(\rho) \; I_o\,(\alpha\rho)\, d\rho \end{cases}$$

and so the general solution of equation (2.5) is obtained in the following form

$$(2.6)\quad \bar{c}(r,p) = -\frac{V}{D}\int_0^r \rho\, c_o(\rho)\left\{ I_o(\alpha r)\; K_o(\alpha\rho) - I_o(\alpha\rho)\; K_o(\alpha r)\right\} d\rho \; + $$

$$+ \; P I_o(\alpha r) + Q \;\; K_o(\alpha r) \;,$$

where the constants P and Q have to be determined from the boundary conditions (2.2) and (2.3). The condition of continuity at r=0 implies Q=0 in view of the logarithmic singularity of $K_o(\alpha r)$ at r=0 . From the condition

$\dfrac{\partial \bar{c}}{\partial r} = 0$ at r=a we obtain

$$P = \frac{V}{D I_o'(\alpha a)} \int_0^a r\, c_o(r) \left\{ I_o'(\alpha a)\; K_o(\alpha r) - I_o(\alpha r)\; K_o'(\alpha a)\right\} dr .$$

Substituting the values of P and Q into (2.6) we find

$$\bar{c}(r,p) = -\frac{V}{D}\left[\int_0^r \rho\, c_o(\rho) \left\{ I_o(\alpha r) \;\; K_o(\alpha\rho) - I_o(\alpha\rho)\; K_o(\alpha r)\right\} d\varphi \; + \right.$$

$$(2.7) \qquad \left. - \frac{I_o(\alpha r)}{I_o'(\alpha a)} \int_0^a r\, c_o(r) \left\{ I_o'(\alpha a)\; K_o(\alpha r) - I_o(\alpha r)\; K_o'(\alpha a)\right\} dr \right] .$$

The inverse of the Laplace transformation (2.4) is given by

(2.8) $$c(r,z) = \frac{1}{2\pi i} \int_L e^{pz} \bar{c}\,(r,p)\, dp ,$$

where L is an arbitrary vertical path $\sigma - i\infty$, $\sigma + i\infty$ in the region of regularity of $\bar{c}(r,p)$ (shaded in fig 1).

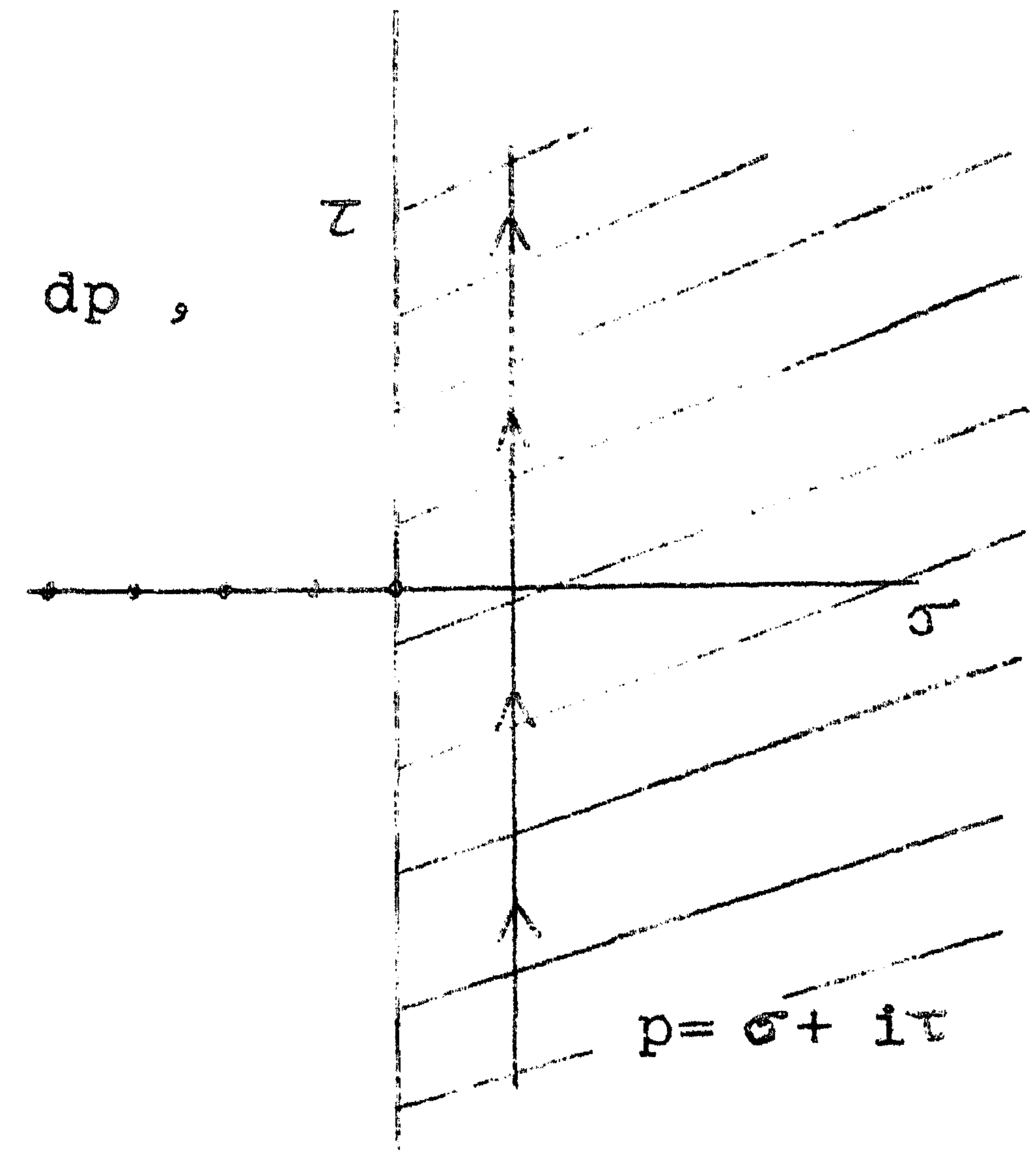

fig 1.

It will be shown in the Appendix, subsection A, that $\bar{c}(r,p)$ is an analytic function of p with a set of simple poles $p_n (n=0,1,2,...)$ at the negative real axis, starting with $p_o=0$. The other poles are obtained from the (simple) zeros of $I_o'(\alpha a)$ (see formula (2.7)) or, which is the same, from

$$J_1(i\alpha a)=0 .$$

The positive zeros of $J_1(x)$ are often called β_n, so the non-trivial zeros of the latter equation may be written as

(2.9) $$\alpha_n = \pm i \beta_n a^{-1}$$

From (2.9) and $\alpha_n^2 = p_n v D^{-1}$ it follows that

(2.10) $$p_n = - \frac{D\beta_n^2}{a^2 v} \qquad n = 1,2,...$$

The origin p=0 must be considered seperately since p=0 is not only a zero of $J_1(x)$ but also a singularity of $K_o(x)$ and $K_o'(x)$.

The zeros of $J_1(x)$ have been tabulated e.g. in [3] and [4].

The right-hand side of (2.8) may now be expressed in a sum of residues

(2.11) $$c(r,z) = \sum_{n=0}^{\infty} \text{Res}\left\{ e^{p_n z}\, \bar{c}(r,p_n)\right\} .$$

In the Appendix(subsection A) a calculation of these residues will be given; here we only mention the formulae

$$\begin{cases} \text{residue at } p_o=0 : & \frac{2}{a^2}\int_0^a r\, c_o(r)\, dr , \\ \text{residue at } p_n : & \frac{2}{a^2} e^{p_n z} \frac{J_o(\frac{r}{a}\beta_n)}{J_o^2(\beta_n)} \int_0^a r\, c_o(r) \cdot \\ & \cdot J_o(\frac{r}{a}\beta_n)\, dr , \quad n=1,2,3,\ldots \end{cases}$$

Combining these results we eventually find

(2.12) $$c(r,z) = \frac{2}{a^2}\left[\int_0^a r\, c_o(r)\, dr + \sum_{n=1}^{\infty} e^{p_n z} \frac{J_o(\frac{r}{a}\beta_n)}{J_o^2(\beta_n)} \cdot \int_0^a r\, c_o(r)\, J_o(\frac{r}{a}\beta_n)\, dr\right],$$

where p_n is given by (2.10).

3. A special case.

Here we consider the case that the concentration at the entrance is described by

(3.1) $$c_o(r) = \begin{cases} 0 & \text{for } 0 \leqslant r \leqslant r_o, \\ 1 & \text{"} \quad r_o \leqslant r \leqslant a . \end{cases}$$

Then the first term of the expansion of $c(r,z)$ reduces to $1-r_o^2 a^{-2}$. Using a certain relation between Bessel functions the integration can be carried out. This will be shown in the Appendix (subsection B), where the following result will be derived

$$\int_0^a r\, c_o(r)\; J_o(\tfrac{r}{a}\beta_n)\; dr = \frac{a r_o}{\beta_n}\; J_1(\tfrac{r_o}{a}\beta_n).$$

The solution of this special problem is therefore given by

$$(3.2)\quad c(r,z) = (1 - \frac{r_o^2}{a^2}) + \frac{2r_o}{a} \sum_{n=1}^{\infty} \frac{e^{p_n z}}{\beta_n} J_1(\frac{r_o}{a}\beta_n)\frac{J_o(\frac{r}{a}\beta_n)}{J_o^2(\beta_n)}$$

The term $1-\frac{r_o^2}{a^2}$, or $\frac{a^2-r_o^2}{a^2}$ describes the situation of ideal mixing at the entrance of the tube. The subsequent terms representing the effect of diffusion and convection are corrections to this picture. In order to obtain a prescribed accuracy it depends on the chosen values of z whether one or more correcting terms must be taken into calculation. For relatively large values of z it suffices to take only one correcting term of the expansion (3.2),

$$(3.3)\quad c(r,z) = (1-\frac{r_o^2}{a^2})+ \frac{2r_o}{a\beta_1} e^{p_1 z} J_1(\frac{r_o}{a}\beta_1)\frac{J_o(\frac{r}{a}\beta_1)}{J_o^2(\beta_1)} + \dots ,$$

where $\beta_1 = 3.8317$ and $p_1 = -\frac{D\beta_1^2}{a^2 v}$.

Appendix.

In this Appendix we give some derivations which are of minor importance to the diffusion problem and which for this reason are omitted in sections 2 and 3.

A. Here we shall give a derivation of the expansion (2.12) of c(r,z). To that purpose we first determine the possible singularities of c(r,p) in the complex p-plane.
The first integral of (2.7) viz.

(A1) $\int_0^r \rho\, c_o(\rho) \left\{ I_o(\alpha r) \;\; K_o(\alpha\rho) - I_o(\alpha\rho)\, K_o(\alpha r) \right\} \, d\varphi$

will be considered first.

We note that $I_o(x)$ is an (even) entire function of x and that $K_o(x)$ has a logarithmic singularity at x=0 of the following kind,

$$K_o(x) = -(\gamma + \ln \tfrac{x}{2})\, I_o(x) + O(x^2) \text{ for } x \to 0,$$

where γ is Euler's constant.
Hence the expression (A1) may have a possible singularity at $\alpha = 0$. However, by considering the behaviour of this expression for $\alpha \to 0$

$$\text{(A2)} \quad \int_0^r \rho\, c_o(\rho) \Big\{ -(\gamma + \ln \tfrac{\alpha\rho}{2})\, I_o(\alpha\rho)\, I_o(\alpha r) + I_o(\alpha r)\, O(\alpha^2) + (\gamma + \ln \tfrac{\alpha r}{2})\, I_o(\alpha r)\, I_o(\alpha\rho) - I_o(\alpha\rho)\, O(\alpha^2) \Big\}\, d\rho,$$

it appears that, with respect to α, the logarithmic terms drop out. Thus (A1) is regular and even with respect to α and consequently also a regular function of p.

We now consider the second integral of (2.7) viz.

$$\frac{v}{D}\, \frac{I_o(\alpha r)}{I_o'(\alpha a)} \int_0^a r c_o(r) \left\{ I_o'(\alpha a)\, K_o(\alpha r) - I_o(\alpha r) K_o'(\alpha a) \right\} dr$$

which may also be written as

$$(A3)\quad \frac{v}{D} I_o(\alpha r) \int_0^a r\, c_c(r) \left\{ K_o(\alpha r) - I_o(\alpha r) \frac{K_o'(\alpha a)}{I_o'(\alpha a)} \right\} dr.$$

It is easily seen that as a funtion of α this expression has a set of poles $\alpha_n = \pm i \beta_n a^{-1}$, or $p_n = -D \beta_n^2 (a^2 v)^{-1}$, due to the zeros of the denominator. The origin must be considered separately. Again it appears that the terms with $\ln \alpha$ disappear, and that (A3) is an even function of α with a pole of the second order in the origin. Thus when considered as a function of p there results a meromorphic function of p with a simple pole in the origin. The residue at p=0 can be calculated by using the following expansions expressing the behaviour for $p \to 0$, or for $\alpha \to 0$,

$$(A4)\quad \begin{cases} I_1(\alpha a) = \frac{\alpha a}{2} + O(\alpha^3) \\ I_o(\alpha r) = 1 + O(\alpha^2) \\ K_o(\alpha r) = -(\gamma + \ln \frac{\alpha r}{2})\, I_o(\alpha r) + O(\alpha^2) \\ K_1(\alpha a) = \quad (\gamma + \ln \frac{\alpha a}{2})\, I_1(\alpha a) + \frac{1}{\alpha a} + O(\alpha) \end{cases}$$

We also use the relations

$$(A5)\quad \begin{cases} I_o'(x) = I_1(x), \\ K_o'(x) = -K_1(x), \end{cases}$$

which may be found, as well as the expansions (A4), in [5] pp. 181 and 182.

Hence for $\alpha \rightarrow 0$ the expansion (A3) may be written as

$$\frac{v}{D}\int_0^a r\, c_o(r)\, I_o(\alpha r)\Big\{ -(\gamma + \ln\frac{\alpha r}{2})\, I_o(\alpha r) + O(\alpha^2) + + (\gamma + \ln\frac{\alpha a}{2})\, I_o(\alpha r) + \frac{\frac{1}{\alpha a} + O(\alpha)}{\frac{\alpha a}{2} + O(\alpha^3)}\, I_o(\alpha r)\Big\}\, dr ,$$

which can be simplified to

$$\frac{v}{D}\int_0^a r\, c_o(r)\Big\{\ln\frac{a}{r} + \frac{2}{(\alpha a)^2} + O(\alpha^2)\Big\}\, dr .$$

From this expression the residue can be derived at once. Using $\alpha^2 = pv\, D^{-1}$ we have

$$\text{(A6).}\quad \underset{p=p_n}{\text{Res}}\,(A3) = \lim_{p\rightarrow 0} e^{pz}\, \frac{v}{D}\int_0^a r\, c_o(r)\Big\{ \ln\frac{a}{r} + \frac{2}{(\alpha a)^2} + + O(\alpha^2)\Big\}\, dr = \frac{2}{a^2}\int_0^a r\, c_o(r)\, dr .$$

The residues at p_n , $n=1,2,3,\ldots$ are found by using

$$\underset{p=p_n}{\text{Res}}\, \frac{1}{I_o'(\alpha a)} = \lim_{p\rightarrow p_n} \frac{p-p_n}{I_o'(\alpha a)} = \frac{1}{\frac{\partial}{\partial p}(I_o'(\alpha a))_{p=p_n}}$$

Since

$$\frac{\partial}{\partial p}(I_o'(\alpha a))_{p=p_n} = \frac{av}{2\alpha_n D}\, I_o''(\alpha_n a) ,$$

we find

$$\underset{p=p_n}{\text{Res}}\, \frac{1}{I_o'(\alpha a)} = \frac{2\alpha_n D}{av\, I_o''(\alpha_n a)} .$$

Taking the residue of (A3) at $p=p_n$ the first term of the integrand vanishes because it is an entire function of α ($\alpha > 0$). The residue is therefore given by

(A7) $$\operatorname*{Res}_{p=p_n} (A3) = - \frac{2\alpha_n e^{p_n Z}}{a} \frac{K_o'(\alpha_n a)\, I_o(\alpha_n r)}{I_o''(\alpha_n a)} \int_0^a r\, c_o(r) \cdot I_o(\alpha_n r)\, dr .$$

We know that $I_o(x)$ satisfies the differential equation

$$y''(x) + \frac{1}{x} y'(x) - y(x) = 0$$

and because $I_o'(\alpha_n a) = 0$ we have the identity

(A8) $$I_o''(\alpha_n a) = I_o(\alpha_n a).$$

Using again the expression of the Wronskian of $I_o(x)$ and $K_o(x)$

$$I_o(x)\, K_o'(x) - I_o'(x)\, K_o(x) = - x^{-1} ,$$

it follows that for $x = \alpha_n a$

(A9) $$I_o(\alpha_n a)\, K_o'(\alpha_n a) = - (\alpha_n a)^{-1} .$$

Using (A8) and (A9) the formula of $\operatorname*{Res}_{p=p_n} (A3)$ becomes

(A10) $$\operatorname*{Res}_{p=p_n} (A3) = \frac{2e^{p_n z}}{a^2} \frac{I_o(\alpha_n r)}{I_o^2(\alpha_n a)} \int_0^a r\, c_o(r)\, I_o(\alpha_n r)\, dr ,$$

$n = 1, 2, \ldots$

Now we consider the closed contour C consisting of the path $\sigma - iR$, $\sigma + iR$ and the semicircle Γ with origin $(\sigma, 0)$ and radius R (fig 2).

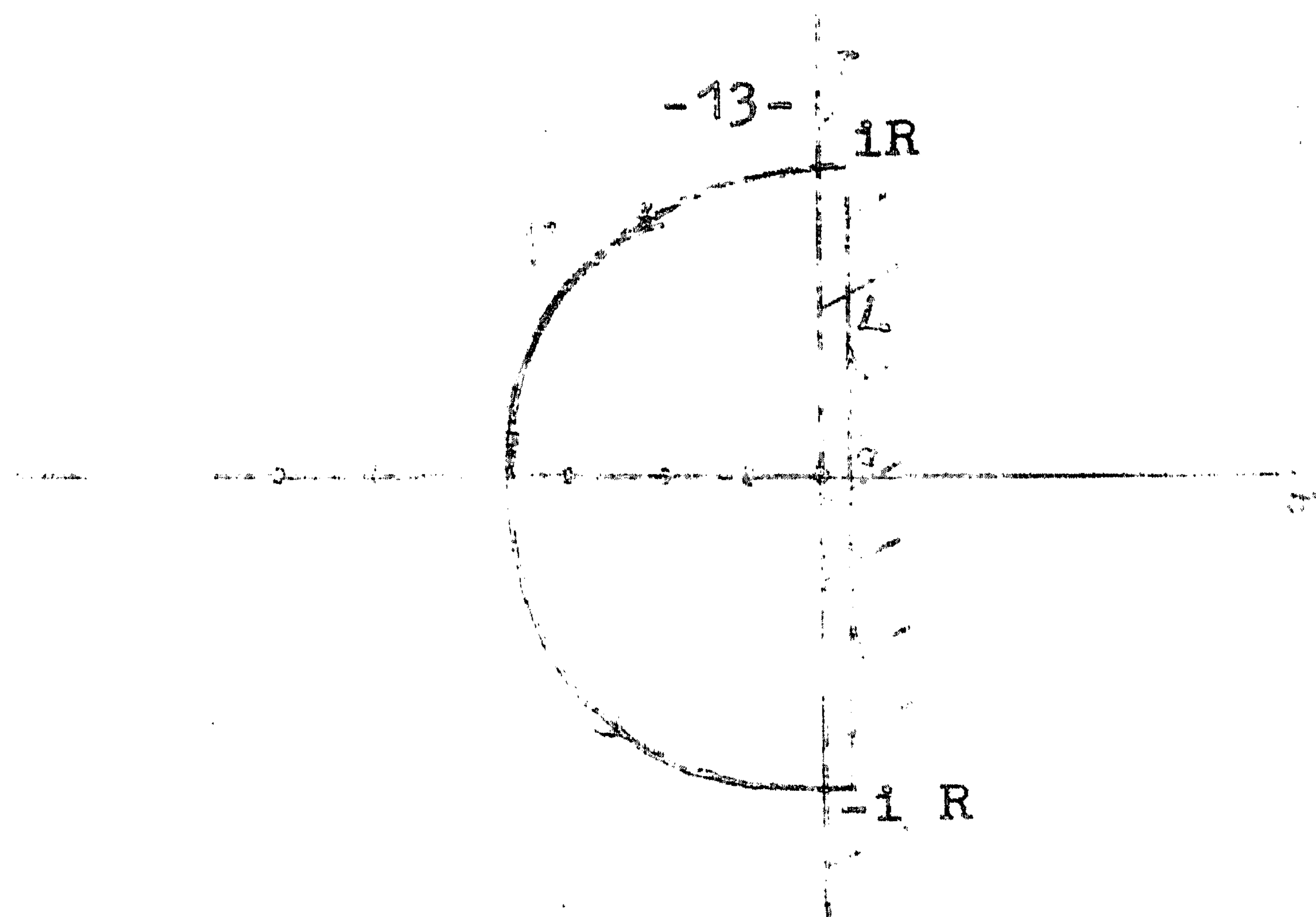

fig.2

If we let $\sigma \rightarrow 0$, leaving a semicircle γ with an arbitrarily small radius ε around the origin and taking care that Γ does not go through any of the poles p_n, it can be shown that

$$\int_{\Gamma} e^{pz} \; \bar{c}\,(r,p)\; dp \rightarrow 0 \qquad \text{for} \quad R \rightarrow \infty \; .$$

In a similar way it appears that

$$\int_{\gamma} e^{pz} \; \bar{c}\,(r,p)\; dp \longrightarrow 0 \qquad \text{for} \quad \varepsilon \longrightarrow 0.$$

Consequently

$$\oint e^{pz} \; \bar{c}\,(r,p)\; dp = \int_{L} e^{pz} \; \bar{c}\,(r,p)\; dp \; ,$$

where L is the vertical path $\sigma - i\infty$, $\sigma + i\infty$ $(\sigma > 0)$.
On the other hand we have the relation

$$\frac{1}{2\pi i} \oint e^{pz} \; \bar{c}\,(r,p)\; dp = \sum_{n=0}^{\infty} \left\{ \text{Res} \quad e^{p_n z} \; \bar{c}\,(r,p_n) \right\} ,$$

and therefore the right-hand side of (2.8) can be written as a sum of residues

$$c(r,z) = \frac{1}{2\pi i} \int e^{pz} \; \bar{c}\,(r,p)\; dp = \sum_{n=0}^{\infty} \left\{ \text{Res} \quad e^{p_n z} \; \bar{c}\,(r,p_n) \right\}.$$

In order to apply this result we combine (A6) and (A10), getting the expansion

$$\text{(A11)}\quad c(r,z) = \frac{2}{a^2}\left[\int_0^a r\,c_o(r)\,dr + \sum_{n=1}^{\infty} e^{p_n z}\,\frac{I_o(\alpha_n r)}{I_o^2(\alpha_n a)}\cdot\int_0^a r\,c_o(r)\,I_o(\alpha_n r)\,dr\right].$$

It is convenient to write this formula in terms of $J_o(ix)$ in place of $I_o(x)$. For that reason we write

$$i\,\alpha_n r = -\frac{r}{a}\beta_n \quad , \quad i\alpha_n a = -\beta_n ,$$

and since $J_o(x)$ is an even function of x, (A11) becomes

$$\text{(A12)}\quad c(r,z) = \frac{2}{a^2}\left[\int_0^a r\,c_o(r)\,dr + \sum_{n=1}^{\infty} e^{p_n}\,\frac{J_o(\frac{r}{a}\beta_n)}{J_o^2(\beta_n)}\cdot\int_0^a r\,c_o(r)\,J_o(\tfrac{r}{a}\beta_n)\,dr\right].$$

B. In section 3 we met with the integral

$$\text{(B1)}\qquad \int_0^a r\,c_o(r)\,J_o(\tfrac{r}{a}\beta_n)\,dr.$$

If $c_o(r)$ is given by (3.1) we may write

$$\text{(B2)}\quad \int_0^a r\,c_o(r)\,J_o(\tfrac{r}{a}\beta_n)\,dr = \int_{r_o}^a r\,J_o(\tfrac{r}{a}\beta_n)\,dr.$$

We use the relation

$$\text{(B3)}\qquad \int_0^x \xi\,J_o(\xi)\,d\xi = -x\,J_o'(x) ,$$

which may easily be verified by differentiating both sides with respect to x. Since $J_o'(x) = -J_1(x)$ it follows that

$$\text{(B4)} \quad \int_a^b x\, J_o(x)\, dx = b\, J_o(b) - a\, J_o(a).$$

Using (B4) the right-hand side of the equation (B2) becomes after some calculations

$$\text{(B5)} \quad \left(\frac{a}{\beta_n}\right)^2 \left\{ \beta_n \; J_1(\beta_n) - \frac{r_o}{a} \beta_n \, J_1\left(\frac{r_o}{a} \beta_n\right) \right\} = \frac{a r_o}{\beta_n} J_1\left(\frac{r_o}{a} \beta_n\right),$$

and so, if $c_o(r)$ be given by (3.1)

$$\int_0^a r\, c_o(r)\, J_o\left(\frac{r}{a} \beta_n\right) dr = \frac{a r_o}{\beta_n} J_1 \left(\frac{r_o}{a} \beta_n\right).$$