STICHTING MATHEMATISCH CENTRUM

2e BOERHAAVESTRAAT 49 AMSTERDAM

AFDELING TOEGEPASTE WISKUNDE

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Mass transport through arcs and flames

by

H. Bavinck



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1. Summary

The transport of particles, caused by axial and radial diffusion and axial flow of convection, will be considered in a d.c.arc and in a laminar flame. The following mathematical model will be discussed. Assuming a steady state in both cases the mass transport may be described in cylindrical coordinates (r,z) by the following partial differential equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\operatorname{Dr}\frac{\partial C}{\partial r}\right) + \frac{\partial}{\partial z}\left(\operatorname{D}\frac{\partial C}{\partial z}\right) - \operatorname{W}\frac{\partial C}{\partial z} = 0, \tag{1.1}$$

where C means the particle concentration, D the coefficient of diffusion, and W the axial velocity. D and W are taken constant; various boundary conditions, corresponding to different approximations of the physical situation, are considered. Solutions of (1.1) are obtained in an explicit form.

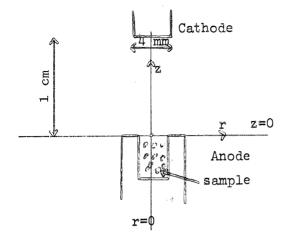
2. Mass transport through a d.c.arc

2.1. Introduction

We shall consider some mathematical models, originating from investigations by Boumans [1] and de Galan [2] concerning the transport of particles through a d.c. arc.

At the lower electrode (the anode), a vapour of an element enters the dischange zone at a rate of Q particles per sec. The vapour consisting of atoms and ions in a proportion depending on the temperature spreads by diffusion (coefficient of diffusion D). Directed transport forces originating from the electric field and the flow of convection cause an additional axial velocity component W acting upwards.

When the steady state is reached, the transport of the atoms and ions through the arc may be described by equation (1.1), where r means the distance to the axis of the arc and z the vertical distance to the anode. Boundary conditions are imposed at the surface of the anode (z = 0) and at the edge of the flame (r = R). Since the arc temperature falls rather



steeply at the edge of the core, we must expect D to drop rapidly as well. A different situation arises for the axial transport velocity W. When ionisation of an element is large in the arc core, W can be shown to decrease rather sharply at the edge of the core. On the other hand if an element ionizes only weakly, W equals the speed of convection, which does

not vary greatly over the arc cross-section.

In this treatment D and W are taken constant. The following boundary conditions may give an acceptable approximation of the physical situation as regards the edge of the core.

- a) As a first approximation the solution of (1.1) is considered in the cylindrical half-space $0 \le r < \infty$, $0 \le z < \infty$ with the boundary condition C = 0 at $r = \infty$. This mathematical model will be discussed in section 2.2. b) Since at distances r > R all atoms and ions have recombined to molecules because of the low temperature, a better boundary condition would be C = 0 at r = R. This approximation can be used for the lower values of the transport velocity W. Since the decrease of D at the edge is ignored, a solution based on it will predict too large mass losses by radial diffusion.
- c) In the hot core of the arc the rate of diffusion is much greater than in the cooler fringe. The low-temperature envelope virtually acts as an impenetrable wall for particles diffusing outward from the core. This may be described by the condition $\frac{\partial C}{\partial r} = 0$ at r = R (R being taken smaller than in the foregoing case). This model may lead to rather good results for large values of the transport velocity W.
- d) As a compromise between the cases b) and c) we may use the condition $\frac{\partial C}{\partial r} hC = 0$ at r = R, where h is a non-negative constant. The case h = 0 corresponds to case c), the case $h = \infty$ to case b). The solutions of (1.1) satisfying this boundary condition will be considered in section 2.3.

At the anode (z = 0) we shall impose the boundary condition that the mass transport through the plane z = 0 vanishes outside the source. In the mathematical model we consider a point source at the origin first and a disk source with the centre at the origin and radius a next.

2.2. Solutions in the cylindrical half-space $0 \le r < \infty$, $0 \le z < \infty$

a) Point source of intensity Q at r = 0, z = 0

Writing $v = \frac{W}{2D}$ in equation (1.1) with constant D and W, the partial differential equation takes the following form

$$\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2} - 2v \frac{\partial C}{\partial z} = 0. \qquad (2.2.1)$$

The boundary conditions are

$$r = 0$$
 $z \neq 0$ C regular, (2.2.2)

$$z = \infty$$
 C bounded, (2.2.3)

$$r = \infty \qquad C = O_a \qquad (2.2.4)$$

$$z = 0 - \frac{\partial C}{\partial z} + 2vC = \frac{Q\delta(r)}{2\pi rD}, (2.2.5)$$

where $\frac{\delta(r)}{2\pi r}$ is the distributional notation of a plane point source at the origin in polar coordinates.

The treatment of this case is similar to that of the problem considered in Lauwerier [3]. The equation (2.2.1) with the conditions (2.2.2), (2.2.3), and (2.2.4) is satisfied by the elementary solution

$$J_0(\lambda r)e^{-z(\sqrt{v^2+\lambda^2-v})}, \qquad (2.2.6)$$

where λ is an arbitrary real parameter. From this we may construct the general solution

$$C(r,z) = \int_0^\infty f(\lambda)J_0(\lambda r)e^{-z(\sqrt{v^2+\lambda^2}-v)}d\lambda. \qquad (2.2.7)$$

The unknown function $f(\lambda)$ has to be determined from condition (2.2.5).

As is well-known a solution of (2.2.1), satisfying the conditions (2.2.2), (2.2.3) and (2.2.4), which describes the effect of a point source of intensity Q at the origin, is given by

$$\frac{Q}{2\pi D} = \frac{e^{-V(\sqrt{z^2 + r^2}^2 - z)}}{\sqrt{z^2 + r^2}}.$$
 (2.2.8)

The latter property may be easily verified by considering the mass transport through a small hemi-sphere around the origin.

From the Laplace transform

$$\int_{b}^{\infty} e^{-pt} J_{0}(a \sqrt{t^{2}-b^{2}}) dt = \frac{e^{-b} \sqrt{p^{2}+a^{2}}}{\sqrt{p^{2}+a^{2}}}$$

(cf. Erdélyi et al., Integral transforms I, 4.15.9) we may derive the following result

$$\int_{0}^{\infty} \frac{\lambda}{\sqrt{\lambda^{2}+v^{2}}} J_{0}(\lambda r) e^{-z(\sqrt{v^{2}+\lambda^{2}}-v)} d\lambda = \frac{e^{-v(\sqrt{z^{2}+r^{2}}-z)}}{\sqrt{z^{2}+r^{2}}}, (2.2.9)$$

which shows that (2,2,8) is of the form (2,2,7).

The boundary condition (2.2.5) suggests the following choice for $f(\lambda)$:

$$f(\lambda) = \frac{Q}{2\pi D} \left[\frac{\lambda}{\sqrt{\lambda^2 + v^2}} - \psi(\lambda) \right], \qquad (2.2.10)$$

where $\psi(\lambda) \rightarrow 0$ for $\lambda \rightarrow \infty$.

This means that C(r,z) is written as

$$C(\mathbf{r},\mathbf{z}) = \frac{Q}{2\pi D} \left[\frac{e^{-\mathbf{v}(\sqrt{\mathbf{z}^2 + \mathbf{r}^2} - \mathbf{z})}}{\sqrt{\mathbf{z}^2 + \mathbf{r}^2}} - \int_0^\infty \psi(\lambda) J_0(\lambda \mathbf{r}) e^{-\mathbf{z}(\sqrt{\mathbf{v}^2 + \lambda^2} - \mathbf{v})} d\lambda \right].$$

From condition (2.2.5) we obtain

$$\int_{0}^{\infty} \psi(\lambda) (\sqrt{v^{2} + \lambda^{2}} + v) J_{0}(\lambda r) d\lambda = v \frac{e^{-vr}}{r}.$$

Using the relation (2,2,9) for z = 0 we find

$$\psi(\lambda) = \frac{\lambda}{\sqrt{\lambda^2 + v^2}} \frac{v}{\sqrt{v^2 + \lambda^2} + v}.$$

Substitution of this expression into (2.2.7) and (2.2.10) gives the following explicit result

$$C(r,z) = \frac{Q}{2\pi D} \int_0^{\infty} \frac{\lambda}{\sqrt{v^2 + \lambda^2} + v} J_0(\lambda r) e^{-z(\sqrt{v^2 + \lambda^2} - v)} d\lambda. \qquad (2.2.11)$$

b) Disk of uniform source density

Next we consider equation (2.2.1) with the conditions (2.2.2), (2.2.3), (2.2.4) and with the additional boundary condition of no mass transport through the plane z=0 outside the disk source of radius a and total intensity Q

$$z = 0$$
, $\frac{\partial C}{\partial z} + 2vC = \frac{Q}{\sqrt{a^2 D}} \theta(a=r)$, (2.2.12)

 $\theta(x)$ being the well-known unit-step function.

First we take a point source of constant intensity Q_0 at the variable point $P(r_0,\phi_0)$ of the plane z=0. The solution is obviously

$$C_1(r,\phi,r_0,\phi_0,z,Q_0) = \frac{Q_0}{2\pi D} \int_0^\infty \frac{\lambda}{\sqrt{v^2+\lambda^2}+v} J_0(\lambda r^*) e^{-z(\sqrt{v^2+\lambda^2}-v)} d\lambda,$$

where $r^{\dagger} = (r^2 + r_0^2 - 2rr_0\cos(\phi - \phi_0))^{\frac{1}{2}}$ is the distance to the translated vertical axis through P_0

In order to obtain the solution for a uniform disk source with total intensity Q and radius a, we may proceed as follows. For each surface element ΔS the contribution to the concentration is $C_1(r,\phi,r_0,\phi_0,z,\frac{Q}{\pi a^2}\Delta S)$.

Thus the total concentration becomes

$$C(r,z) = \int_{0}^{a} \int_{0}^{2\pi} \frac{Q}{\pi a^{2}} r_{0} dr_{0} d\phi \frac{1}{2\pi D} \int_{0}^{\infty} \frac{\lambda}{\sqrt{v^{2} + \lambda^{2}}} J_{0}(\lambda r^{\dagger}) e^{-z(\sqrt{v^{2} + \lambda^{2}}} - v)_{d\lambda}.$$

Using the addition formula (Watson [4], 4.82)

$$J_{0}(\lambda \sqrt{r^{2}+r_{0}^{2}-2rr_{0}\cos(\phi-\phi_{0})}) = J_{0}(\lambda r)J_{0}(\lambda r_{0}) + 2\sum_{m=1}^{\infty} J_{m}(\lambda r)J_{m}(\lambda r_{0})\cos m(\phi-\phi_{0})$$

we obtain

$$C(r,z) = \frac{Q}{\pi a^{2}D} \int_{0}^{\infty} \frac{\lambda}{\sqrt{v^{2}+\lambda^{2}}+v} e^{-z(\sqrt{v^{2}+\lambda^{2}}-v)} J_{0}(\lambda r) (\int_{0}^{a} r_{0}J_{0}(\lambda r_{0})dr_{0})d\lambda$$

$$= \frac{Q}{\pi aD} \int_{0}^{\infty} \frac{J_{1}(\lambda a)}{\sqrt{v^{2}+\lambda^{2}}+v} J_{0}(\lambda r) e^{-z(\sqrt{v^{2}+\lambda^{2}}-v)} d\lambda. \qquad (2.2.13)$$

The former result (2.2.11) can be recovered from (2.2.13) by taking the limit for $a \rightarrow 0$.

2.3. Solutions satisfying the boundary condition $\frac{\partial C}{\partial r}$ - hC = 0 at r = R

It is convenient to introduce the following dimensionless variables:

$$r = r R_0$$
 $z = z R_0$ $v = \frac{WR}{2D}$, $a = a R_0$

Substitution in equation (1.1) leads to

$$\frac{\partial^{2}C}{\partial r^{+2}} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^{2}C}{\partial z^{+2}} - 2v \frac{\partial C}{\partial z^{+}} = 0.$$
 (2.3.1)

For the sake of simplicity the asterisks will be omitted from now on.

a) Point source of intensity Q at z = 0, r = 0

In this section the solution of (2.3.1) will be derived with the following boundary conditions:

$$r = 0$$
 $z \neq 0$ C regular, (2.3.2)

$$z = \infty$$
 C bounded, (2.3.3)

$$r = 1 \qquad \frac{\partial C}{\partial r} - hC = 0, \qquad (2.3.4)$$

$$z = 0 - \frac{\partial C}{\partial z} + 2vC = \frac{Q\delta(r)}{2\pi rRD}, (2.3.5)$$

In order that the elementary solution (2.2.6) satisfies the condition (2.3.4) λ must be a root of

$$\lambda J_1(\lambda) = hJ_0(\lambda) = 0. \qquad (2.3.6)$$

It is known (see Watson [4] 15.25), that equation (2.3.6) has no complex roots and that there are an infinite number of real roots $+\alpha_1$, $+\alpha_2$, $+\alpha_3$, $+\alpha_3$, $+\alpha_5$ of for all j). For a number of values of h, the first few α_n are tabulated in [5], table III.

The general solution of (2.3.1) satisfying (2.3.2), (2.3.3) and (2.3.4) may be written as

$$C(r,z) = \sum_{n=1}^{\infty} c_n J_0(r\alpha_n) e^{-z(\sqrt{v^2 + \alpha_n^2} - v)}.$$
 (2.3.7)

The unknown coefficients c_n have to be determined from condition (2.3.5).

It is well-known that the functions $J_0(r\alpha_n)$ form a complete orthogonal set (see [5], page 172), in the sense that $\int_0^1 J_0(r\alpha_n)J_0(r\alpha_m)$ rdr = 0 if $m \neq n$.

This suggests the following distributional expansion of $\frac{\delta(r)}{r}$:

$$\frac{\delta(\mathbf{r})}{\mathbf{r}} = \sum_{n=1}^{\infty} a_n J_0(\mathbf{r}\alpha_n).$$

The coefficients $\mathbf{a}_{\mathbf{n}}$ can formally be calculated from

$$\frac{1}{2} \left\{ J_0^2(\alpha_n) + J_1^2(\alpha_n) \right\} a_n = \int_0^1 \delta(r) J_0(r\alpha_n) dr = 1,$$

which gives

$$a_n = \frac{2}{J_0^2(\alpha_n) + J_1^2(\alpha_n)}$$
, $n = 1, 2, 3, ...$

Imposing condition (2.3.5) on the solution (2.3.7) and equating the corresponding terms of the series (which may be done because of the completeness of the set $\{J_0(r\alpha_n)\}$) we obtain

$$c_{n}(\sqrt{v^{2}+\alpha_{n}^{2}}-v)J_{0}(r\alpha_{n})+2c_{n}vJ_{0}(r\alpha_{n})=\frac{Q}{\pi RD}\frac{1}{J_{0}^{2}(\alpha_{n})+J_{1}^{2}(\alpha_{n})}J_{0}(r\alpha_{n})$$

so that

$$c_n = \frac{Q}{\pi RD} \frac{1}{(\sqrt{v^2 + \alpha_n^2 + v})} \frac{1}{J_0^2(\alpha_n) + J_1^2(\alpha_n)}, \quad n = 1, 2, 3, \dots (2.3.8)$$

Substitution in (2.3.7) gives the required explicit expression

$$C(r,z) = \frac{Q}{\pi RD} \sum_{n=1}^{\infty} \frac{1}{\sqrt{v^2 + \alpha_n^2} + v} \frac{1}{J_0^2(\alpha_n) + J_1^2(\alpha_n)} J_0(r\alpha_n) e^{-z(\sqrt{v^2 + \alpha_n^2} - v)} .(2.3.9)$$

b) Uniform disk source of radius a and total intensity Q

Here we have equation (2.3.1) with the boundary conditions (2.3.2), (2.3.3) and (2.3.4) with the additional condition:

$$z = 0 \qquad -\frac{\partial C}{\partial z} + 2vC = \frac{Q}{\pi a^2 DR} \theta(a-r). \qquad (2.3.10)$$

The expansion of $\theta(a-r)$ in the set $\{J_0(r\alpha_n)\}$ is

$$\theta(a=r) = \sum_{n=1}^{\infty} b_n J_0(r\alpha_n),$$

where

$$b_{n} = \frac{2aJ_{1}(a\alpha_{n})}{\alpha_{n}\{J_{0}^{2}(\alpha_{n})+J_{1}^{2}(\alpha_{n})\}}, n = 1,2,3,\dots$$

The solution of (2.3.1) may be written in the form (2.3.7) again. Following the same procedure as in the preceding case we find

$$C(r_{0}z) = \frac{2Q}{\pi aDR} \sum_{n=1}^{\infty} \frac{1}{\sqrt{v^{2} + \alpha_{n}^{2}} + v} \frac{J_{1}(a\alpha_{n})}{\alpha_{n} \{J_{0}^{2}(\alpha_{n}) + J_{1}^{2}(\alpha_{n})\}} J_{0}(r\alpha_{n}) e^{-z(\sqrt{v^{2} + \alpha_{n}^{2}} - v)}.$$
(2.3.11)

3. Mass transport through a laminar flame

3.1. Introduction

In the homogeneous hot part of a laminar flame a small pearl of an element is suspended by a platinum wire. The material is spread by diffusion and convection (due to the air convection and the gas stream). In order to give a mathematical description of the mass transport through the flame, we consider a cylindrical coordinate system, where the pearl is reduced to a point source of intensity Q at the origin. The z-axis is chosen along the axis of the flame; r means the distance to the z-axis.

The mass transport is described by equation (1.1), if a steady state is assumed.

If we restrict ourselves to not too large values of r and |z| the axial velocity component due to the convection W may be regarded as constant, whereas the coefficient of diffusion D may be considered independent of z. In the mathematical model treated here D and W are chosen constant. As in section 2.3 we try to compensate the neglect of the radial decrease of D by imposing the boundary condition $\frac{\partial C}{\partial r} - hC = 0$ at r = R at the edge of the flame, where h is a certain non-negative parameter, the value of which has to be determined experimentally.

Introduction of dimensionless variables in the same way as in section 2.3 leads to the following partial differential equation and boundary conditions:

$$\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2} - 2v \frac{\partial C}{\partial z} = 0, \qquad (3.1.1)$$

$$z = + \infty$$
 C bounded, (3.1.2)

$$r = 0$$
 $z \neq 0$ C regular, (3.1.3)

$$r = 1 \qquad \frac{\partial C}{\partial r} - hC = 0, \qquad (3.1.4)$$

$$r = 0$$
 $z = 0$ $C \sim \frac{Q}{4\pi DR \sqrt{z^2 + r^2}}$ (3.1.5)

3.2. Derivation of the solution

This problem will be solved by using two-sided Laplace transformation. The solution of equation (3.1.1) with diffusion from a point source of intensity Q at the origin with diffusion in the whole space $-\infty < z < \infty$, $0 < r < \infty$ is well known, viz.

$$C_0(r,z) = \frac{Q}{4\pi RD} \frac{e^{-v(\sqrt{z^2+r^2} - z)}}{\sqrt{z^2+r^2}}$$
.

The constant Q is equal to the mass transport through a small sphere around the origin.

Therefore we take

$$C(r,z) = \frac{Q}{4\pi DR} \frac{e^{-V(\sqrt{z^2+r^2}-z)} + C^*(r,z)}{\sqrt{z^2+r^2}} + C^*(r,z).$$
 (3.2.1)

Two-sided Laplace transformation $\overline{C}^* = \int_{-\infty}^{+\infty} e^{-pz} C^* dz$ applied on equation (3.1.1) yields

$$\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} - q^2 C = 0, \qquad (3.2.2)$$

where $q^2 = 2pv = p^2$.

The boundary conditions become

$$r = 0$$
 \overline{C}^* regular, (3.2.3)

$$\mathbf{r} = 1 \qquad \frac{\partial \mathbf{C}}{\partial \mathbf{r}} - \mathbf{h} \mathbf{C}^{\dagger} = -\frac{\mathbf{Q}}{2\pi \mathbf{D} \mathbf{R}} \left[\mathbf{q} \mathbf{K}_{0}^{\dagger}(\mathbf{q}) - \mathbf{h} \mathbf{K}_{0}(\mathbf{q}) \right]. \qquad (3.2.4)$$

We have used here, after the substitution x = i(p - v), the relation

$$\int_0^\infty \cos(xy) \frac{\exp(-\beta \sqrt{x^2 + \alpha^2})}{\sqrt{x^2 + \alpha^2}} dx = K_0(\alpha \sqrt{\beta^2 + y^2})$$

(cf. Erdélyi, Integral transforms I, 1.4.(27)).

The solutions of (3.2.2) are linear combinations of the modified Bessel functions $I_0(qr)$ and $K_0(qr)$. Because of condition (3.2.3) we may take

$$\overline{C}^* = A I_0(qr)$$

Application of condition (3.2.4) gives

$$A\left[qI_0^{\dagger}(q) - hI_0(q)\right] = -\frac{Q}{2\pi DR} \left[qK_0^{\dagger}(q) - hK_0(q)\right],$$

Hence

$$\overline{C} = -\frac{Q}{2\pi DR} \frac{qK_0^{\theta}(q) - hK_0(q)}{qI_0^{\theta}(q) - hI_0(q)} I_0(qr)$$

and

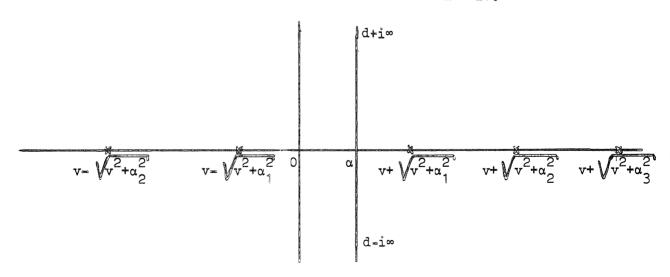
$$\overline{C}(r_{p}) = \frac{Q}{2\pi DR} \frac{K_{0}(qr)[qI_{0}^{\dagger}(q)-hI_{0}(q)] - I_{0}(qr)[qK_{0}^{\dagger}(q)-hK_{0}(q)]}{qI_{0}^{\dagger}(q) - hI_{0}(q)}.$$

The nummerator is a regular function of p, because the logarithmic parts cancel. In addition, both nummerator and denominator are even functions of $q = \sqrt{2pv - p^2}$, which means that there are no branch points.

We now apply the inversion formula for Laplace transforms:

$$C(r,z) = \frac{1}{2\pi i} \int_{d-i\infty}^{d+i\infty} e^{pz} \ \overline{C}(r,p) dp, \text{ holding at least for}$$

$$0 < d < 2v.$$



The poles of the integrand are situated at the points $\sqrt{p^2-2pv}=\alpha_n$ or $p=v\pm\sqrt{v^2+\alpha_n^2}$, where the numbers $\{\alpha_n\}$ satisfy equation (2.3.6). For positive values of z we are closing the path of integration by means of a large semicircle to the left. The contribution of this semicircle to the integral tends to zero.

Taking the residues of the denominator and using the relation $I_0(z)K_0^*(z)=I_0^*(z)K_0(z)=-\frac{1}{z}$ (see Watson [4], 3.71 (19)) and the fact that the numbers $\{\alpha_n\}$ satisfy (2.3.6), we finally obtain

$$C(r,z) = \frac{Q}{2\pi DR} \sum_{n=1}^{\infty} \frac{1}{\sqrt{v^2 + \alpha_n^2}} \frac{1}{J_0^2(\alpha_n) + J_1^2(\alpha_n)} J_0(r\alpha_n) e^{-z(\sqrt{v^2 + \alpha_n^2} - v)}, z > 0.$$
(3.2.5)

For negative values of z we close the path of integration by means of a large semicircle to the right. We easily find

$$C(r,z) = \frac{Q}{2\pi DR} \sum_{n=1}^{\infty} \frac{1}{\sqrt{v^2 + \alpha_n^2}} \frac{1}{J_0^2(\alpha_n) + J_1^2(\alpha_n)} J_0(r\alpha_n) e^{z(\sqrt{v^2 + \alpha_n^2}^2 + v)}, z < 0.$$
(3.2.6)

For small values of |z| the convergence of the right-hand sides of (3.2.5) and (3.2.6) is very slow. However, in the region of physical interest the convergence is satisfactory.

References

- [1] P.W.J.M. Boumans, Introduction to Fundamental Theory of Spectrochemical Analysis, with special reference to the DC Carbon Arc (1965-1966).
- [2] L. de Galan, Particle distribution in the d.c. carbon arc (thesis, Amsterdam 1965).
- [3] H.A. Lauwerier, Diffusion from a point source into a space bounded by an impenetrable plane, Appl. Sci. Res. A6 (197-204).
- [4] G.N. Watson, A treatise on the theory of Bessel functions.
- [5] H.S. Carslaw and J.C. Jaeger, Conduction of heat in solids.