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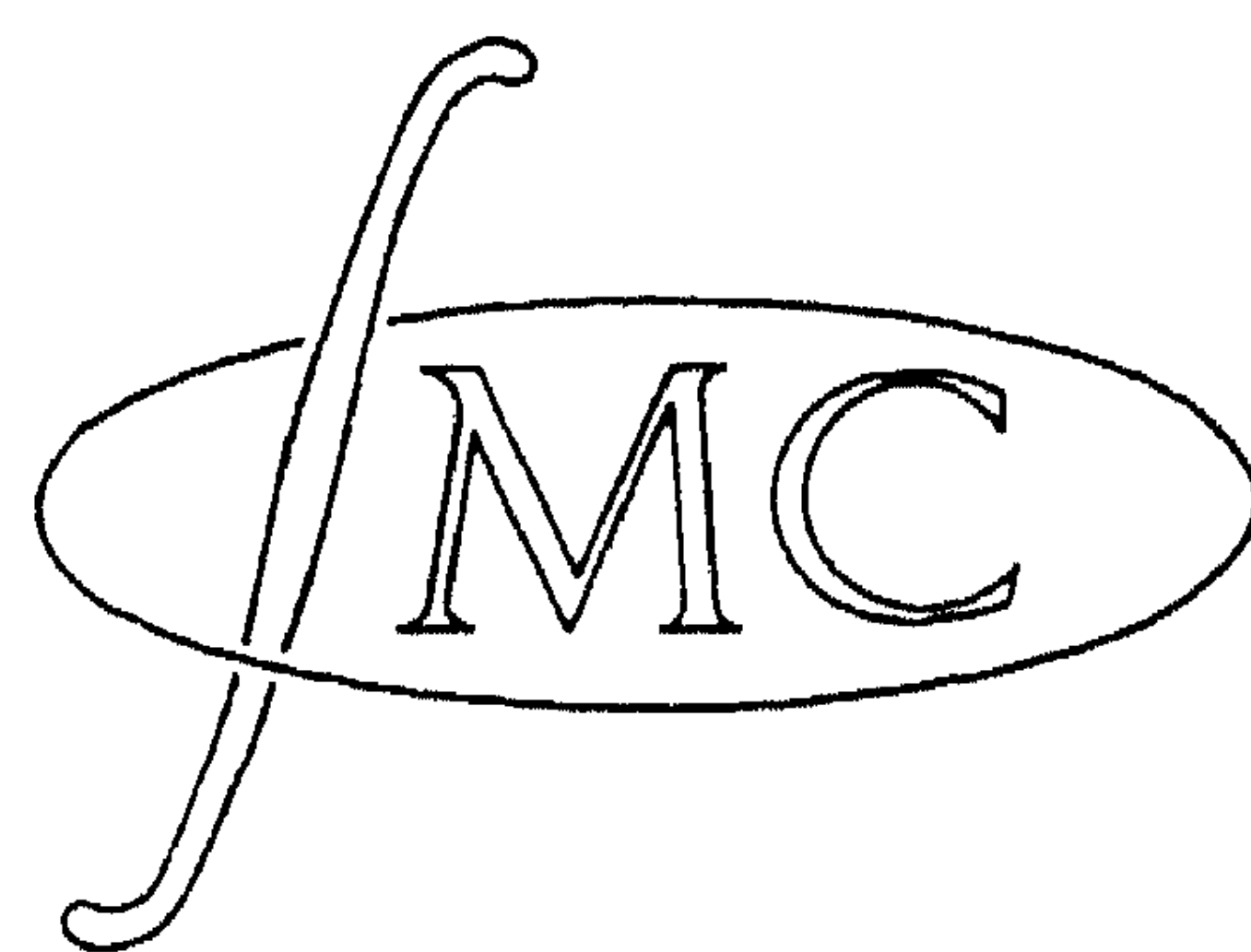
AFDELING TOEGEPASTE WISKUNDE

Technical Note TN 38

On the absorption by homogeneous
spherical particles

by

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§ 1. Introduction.

In TN 37 "Diffusion in layered media" we investigated the absorption of material by a layered sphere surrounded by a reservoir containing the material to be absorbed.

In that paper we assumed that the concentration of the material in the reservoir (e.g. a solution of the material) does not change during the absorption process. This assumption however is only valid, when the amount of absorbed material is small in comparison with the material present in the reservoir. In most practical cases the concentration of the material in the reservoir will change due to the absorption by the sphere and therefore it is not allowed to make the assumption of constant concentration at the surface. There will therefore be a complication in the boundary condition to be posed for the concentration at the surface of the sphere. This change in the boundary condition makes the determination of the amount of material absorbed by the sphere rather cumbersome in case the sphere is layered.

However, it seems that this problem upto now has not even been treated for a homogeneous sphere. In this technical note we shall solve this problem.

The following may be said about the experimental background. To determine the rate at which radioactive material in solution is absorbed by mudparticles or other particles suspended in the liquid, a certain amount of mud is brought into bulbs containing radioactive material in aqueous solution and a suspension is made by shaking. After some time the amount of radioactive material absorbed by the particles is measured and from these measurements the diffusion constant characterizing the speed of the diffusion is to be determined.

We shall derive a formula for the amount of material absorbed by a number of equal homogeneous spheres as a function of time; this formula contains a.o. the diffusion constant, characterizing the speed of the diffusion, as a parameter. By means of this formula and the measured amount of absorbed material, the diffusion constant of e.g. the mud particles can be determined.

The experiments are carried out by Dr. E.K.Duursma of the "Ned. Inst. voor Onderzoek der Zee", who also posed the above problem to us.

In section 2 the equations, boundary conditions and initial value conditions are set up and some further important formulae are given. In section 3 the equations are solved.

§2. Equations, conditions and other formulae.

We consider a volume V containing on the one hand an aqueous solution of (radioactive) material with concentration, say, 1 and on the other hand N equal homogeneous spherical particles all with radius R , which absorb material from the solution.

We introduce coordinates r and t , where r is the distance from the centre of a particle and t the time; the concentration of absorbed material in a particle is denoted by $C(r,t)$ with $0 \leq r \leq R$ and $0 < t < \infty$. We assume that at $t=0$ all the material is in the solution and so $C(r,0)=0$.

If the diffusion constant of the particles is given by D , the function $C(r,t)$ satisfies the following differential equation:

$$D\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r}\right)C(r,t) = \frac{\partial C(r,t)}{\partial t}, \quad (0 \leq r \leq R, 0 < t), \quad (2.1)$$

with the initial condition

$$C(r,t) = 0 \quad \text{for} \quad t=0 \quad \text{and} \quad 0 \leq r \leq R, \quad (2.2)$$

and the boundary conditions

$$C(r,t) = C_S(t) \quad \text{for} \quad r=R \quad \text{and} \quad 0 \leq t \leq \infty, \quad (2.3)$$

and

$$C(r,t) = \text{finite} \quad \text{for} \quad r=0 \quad \text{and} \quad 0 \leq t \leq \infty, \quad (2.4)$$

where $C_S(t)$ is the concentration of the material in the solution. This quantity C_S will change due to the absorption in the following way. The amount of material absorbed by the N spheres in t seconds is

$$M(t) = 4 \pi R^2 N D \int_0^t \frac{\partial C(R,\tau)}{\partial r} d\tau, \quad (2.5)$$

and hence the concentration C_S of the material in the solution at time t is given by the expression

$$C_S = 1 - \rho D \int_0^t \frac{\partial C(R, \tau)}{\partial r} d\tau \quad (2.6)$$

with

$$\rho = \frac{4\pi R^2 N}{V - 4/3\pi R^3 N} \quad (2.7)$$

Hence the boundary condition (2.3) is given by the equation

$$C(R, t) = 1 - \rho D \int_0^t \frac{\partial C(R, \tau)}{\partial r} d\tau. \quad (2.8)$$

The boundary value problem, defined by the equations (2.1), (2.2), (2.4) and (2.8), will be solved with the aid of the Laplace-transformation, viz.

$$\bar{C}(r, p) = \int_0^\infty e^{-pt} C(r, t) dt. \quad (2.9)$$

Introducing the function

$$E(r, t) = r C(r, t), \quad (2.10)$$

the Laplace transform of E satisfies the differential equation

$$\frac{\partial^2 \bar{E}(r, p)}{\partial r^2} = q^2 \bar{E}(r, p), \quad (2.11)$$

with

$$q = \sqrt{\frac{p}{D}}. \quad (2.12)$$

The boundary conditions are

$$\bar{E}(R,p) = \frac{1}{p} \left[R - \rho D \left\{ \frac{\partial \bar{E}(R,p)}{\partial r} - \frac{1}{R} \bar{E}(R,p) \right\} \right], \quad (2.13)$$

$$\bar{E}(0,p) = 0.$$

The quantity we are interested in is the total amount of material absorbed namely $M(t)$. The Laplace transform of this quantity reads as

$$\bar{M}(p) = 4\pi N \frac{D}{p} \left\{ R \frac{\partial \bar{E}(R,p)}{\partial r} - \bar{E}(R,p) \right\} \quad (2.14)$$

After solving (2.11) with the condition (2.13) and substituting the result into (2.14) we obtain the transform $\bar{M}(p)$. Applying the inverse Laplace transformation we finally get the function $M(t)$.

§3. Solution of the problem.

The general solution of equation (2.11) is

$$\bar{E}(r,p) = A \operatorname{ch} qr + B \operatorname{sh} qr, \quad (3.1)$$

and application of the boundary conditions (2.13) leads to the formula

$$\bar{E}(r,p) = \frac{R^2 \operatorname{sh} qr}{pR \operatorname{sh} qR + \rho D \{qR \operatorname{ch} qR - \operatorname{sh} qR\}} \quad (3.2)$$

Substituting (3.2) into (2.14) we get

$$\bar{M}(p) = \frac{4\pi R^2 DN}{p} \left[\frac{qR \operatorname{ch} qR - \operatorname{sh} qR}{pR \operatorname{sh} qR + \rho D \{qR \operatorname{ch} qR - \operatorname{sh} qR\}} \right]. \quad (3.3)$$

The relevant quantity $M(t)$ is obtained by means of the inversion integral

$$M(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} \bar{M}(p) dp. \quad (3.4)$$

The path of integration, a line parallel to the imaginary axis and on the right hand side of the singularities of the integrand, is closed with a large semicircle to the left, not passing through points where the integrand is singular. This can be done because of the fact that the integrand has no branch points. This extension of the path of integration gives no contribution to the integral as the radius of this semicircle tends to infinity and Cauchy's theorem gives the result as the sum of the residues of the integrand in the poles. The pole $p = 0$ gives the stationary state, viz.

$$M(t=\infty) = \frac{4}{3} \pi R^3 N \frac{1}{1 + \frac{\rho R}{3}}. \quad (3.5)$$

Further contributions to $M(t)$ come from the poles of the integrand, the location of which is found from the transcendental equation

$$\Delta = pR \operatorname{sh} qR + \rho D qR \operatorname{ch}\{qR - \operatorname{sh} qR\} = 0. \quad (3.6)$$

We put

$$qR = i\sigma,$$

so that

$$p = -\frac{D}{R^2} \sigma^2,$$

and we obtain

$$-\frac{DR}{R^2} \sigma^2 i \sin \sigma + \rho D \{i\sigma \cos \sigma - i \sin \sigma\} = 0$$

or

$$\operatorname{tg} \sigma = \frac{\rho R \sigma}{\sigma^2 + \rho R}. \quad (3.7)$$

In order to find a good approximation for the roots of this equation we suppose that

$$\rho R \ll 1 \quad (3.8)$$

or according to (2.7)

$$\frac{4\pi R^3 N}{V - 4/3\pi R^3 N} \ll 1. \quad (3.9)$$

The physical meaning of this assumption is simply that the ratio of the total volume V_P of the spherical particles and the volume V is small, or more precisely

$$\frac{V_P}{V} \ll \frac{1}{4}. \quad (3.10)$$

Since this is certainly true in most cases of practical interest, the condition (3.8) is not a severe restriction.

With this assumption the roots of the equation (3.7) are approximately given by

$$\sigma_n - n\pi \approx \operatorname{tg} \sigma_n = \frac{\rho R \sigma_n}{\sigma_n^2 + \rho R}$$

or

$$\sigma_n \approx n\pi \left(1 + \frac{\rho R}{n^2 \pi^2} \right) \quad (n = 1, 2, 3, \dots) \quad (3.11)$$

The residues sought for are found by substituting these values of σ into

$$\frac{4\pi R^2 ND}{p} \cdot \frac{2Dq}{\frac{d\Delta}{dq}} \{qR \operatorname{ch} qR - \operatorname{sh} qR\} \exp [q^2 Dt] .$$

The residue R_n in the pole corresponding with $\sigma_n = n\pi \left(1 + \frac{\rho R}{n^2 \pi^2} \right)$ is therefore approximated by

$$R_n = \frac{-8R^3 \left(1 - \frac{5\rho R}{n^2 \pi^2} \right)}{n^2 \pi} \exp \left[- \frac{Dn^2 \pi^2 \left(1 + \frac{\rho R}{n^2 \pi^2} \right)^2 t}{R^2} \right] \quad (3.12)$$

Summing the residues we finally obtain the approximate result

$$M(t) \approx \frac{4}{3} \pi R^3 N \left[\frac{1}{1 + \frac{\rho R}{3}} - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{\left(1 - \frac{5\rho R}{n^2 \pi^2} \right)}{n^2} \exp \left[- \frac{Dn^2 \pi^2 \left(1 + \frac{\rho R}{n^2 \pi^2} \right)^2 t}{R^2} \right] \right] \quad (3.13)$$

It is again stressed that this result is only valid when the physical assumption (3.10) is satisfied and the result is the more accurate according as there are less particles contained in the solution. If ρ tends to zero the formula (3.13) tends to the wellknown exact solution valid for the case that a constant concentration 1 for the material in the liquid is assumed. (J. Crank, Mathematics of diffusion 1956 p.86 formula (6.20)).

As was remarked earlier the stationary solution $M(\infty)$ is given by the residue in the pole $p=0$ and it is represented by the first term of (3.13), viz.

$$\begin{aligned} M(\infty) &= \frac{4}{3} \pi R^3 N \cdot \frac{1}{1 + \frac{\rho R}{3}} \\ &= \frac{4}{3} \pi R^3 N \cdot \frac{V - 4/3 \pi R^3 N}{V} . \end{aligned} \quad (3.14)$$

This result is in accordance with the fact that at $t=\infty$ the concentration is that of a homogeneous distribution in a volume V of material that originally was contained in a volume $V - \frac{4}{3}\pi R^3 N$.