

Recommendations for

The presentation of plastics design data —

Part 5: Other properties —

Section 5.5: Data on diffusion

IMPORTANT NOTE. Before reading this Recommendation it is essential to read the General Introduction to this series of recommendations, issued separately.

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Summary of pages

This document comprises a front cover, an inside front cover, pages i and ii, pages 1 to 8 and a back cover.

This standard has been updated (see copyright date) and may have had amendments incorporated. This will be indicated in the amendment table on the inside front cover.

Amendments issued since publication

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The following BSI references relate to the work on this standard:
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Introduction

This section gives guidance on diffusion and the following associated phenomena as related to plastics materials.

- a) *Sorption*, where the following are covered:
 - 1) rates of absorption and desorption and derived diffusion data;
 - 2) equilibrium sorption, solubility.
- b) *Permeability*, where the following are covered:
 - 1) steady-state measurements, covering permeability coefficients for homogeneous barriers and transmission rates for heterogeneous systems and for particular barriers;
 - 2) diffusion coefficients from non-steady states.

Diffusion describes the translational movement of a molecular species in a continuous phase; it is frequently a process which occurs to equalize concentrations in a single phase. As mentioned above, associated with diffusion are several phenomena of technological importance, for example, absorption and desorption of fluids (gases and liquids) by plastics, and permeation of films and thicker sections by fluid penetrants. Exceptionally a solid may diffuse into a plastics matrix.

Absorption and desorption describe the entry into, or exit from, a plastics material by a fluid penetrant, defining these processes as non steady-state processes. The equilibrium state of maximum absorption (reached theoretically only after infinite time) is the solubility of the fluid in the plastics material. It is possible that contact with a penetrant may result in the leaching of a component from the plastics; this may result in contamination.

Permeation of plastics of thick section by penetrants with low rates of diffusion may take such a long time to attain the steady state that account must be taken of these non-steady conditions in design.

The rate of diffusion is defined as the amount of substance passing perpendicularly through a reference surface of unit area during unit time. Classical diffusion theory is based on Fick's first law which states that the amount of material Q passing normally through a given plane of unit area in unit time is proportional to the concentration gradient at that plane $\frac{dc}{dx}$. Mathematically, this is defined by the expression:

$$Q = -\frac{Ddc}{dx} \quad (1)$$

where c is the concentration of diffusion material,

x is the dimension in the direction normal to the plane, and

D is a constant, the diffusion coefficient.

It can readily be shown for diffusion taking place only in the x direction that the following expression applies:

$$\frac{dc}{dt} = \frac{Dd^2c}{dx^2} \quad (2)$$

where t is the time.

This is Fick's second law of diffusion, derived on the assumption that D is constant. The assumption that D is independent of concentration and of the position co-ordinates is a special case and is not generally valid. There is no particular difficulty in formulating the equations if D is not constant but application of the equations to physical measurement is inconvenient. When the diffusion coefficient is dependent on the concentration but does not depend explicitly on the position co-ordinates, mathematical analysis allows the determination of differential diffusion coefficients, employing the equations for constant D within sufficiently small concentration ranges so that the variation of D within these concentration ranges is small compared with D .

The diffusion coefficient is temperature dependent and if the activation energy is known, the data for diffusion controlled processes can be extrapolated from one temperature to another. Care must be taken, however, that such extrapolation is justifiable.