**INTRODUCTION TO PROBLEM**

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Steady state diffusion

Diffusion refers to the net movement of a species down a concentration gradient, from an area of high concentration to an area of low concentration. Importantly, diffusion can take place in any phase of matter, including in solids! Steady state (time independent) diffusion is described by Fick’s first law:

A black and white math equation

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Here, JJ is the diffusion flux: the rate at which an amount of a substance passes through a surface area. DD is the diffusion coefficient, which is sometimes called diffusivity. It depends on the specific circumstances the diffusion is occurring in, including what materials are involved and the state of the surrounding environment. Finally, here C is concentration   
(M or , so  is the change in concentration with respect to change in position)

Therefore, Fick's first law tells us how concentration change flows over the region between two different concentrations.

A diagram of a function

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Diffusion coefficient

Diffusion is a thermally activated process, and the temperature dependence is reflected in the diffusion coefficient. The diffusion coefficient (diffusivity) is also described by an Arrhenius relationship! Picture an atom diffusing through a crystalline solid: it must move through the lattice. One way this can happen is, if the atom is sufficiently small, it can travel hop from interstitial site to interstitial site. Larger atoms can diffuse, too, but it’s a more energy-consuming process. One mechanism for this to happen is if a vacancy is first created in the lattice, and then the diffusing atom moves into the now-vacant lattice site. As vacancies diffuse through the lattice, other species can follow. Of course, there are more moving parts with this process, and more energy is required.

The energy required for diffusion to occur can be thought of as an activation energy. The diffusion coefficient is:

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Here, D0 is the maximum value of diffusivity, 𝐸𝑎 is the activation energy, kB𝑘𝐵 is the Boltzmann constant, and T𝑇 is temperature. By describing the diffusion coefficient with an Arrhenius relation, recall that we are saying that at a given temperature, T𝑇, the ratio of the thermal energy given by 𝑘𝐵𝑇 to the activation energy 𝐸𝑎 sets the value of the diffusion coefficient, and it is maximized at infinite temperature.

Fick’s second law

If the concentration profile varies with respect to time, the steady-state assumption no longer holds, and instead *Fick’s second law* is used instead:

A black and white math equation

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Solutions to Fick’s second law are of the form:

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Here, Cs is the concentration of the source, C0 is the initial concentration, 𝐶(𝑥, 𝑡) is the expression for concentration as a function of position and time, D is the diffusion coefficient, and **erf** is the error function.

Transition to 2D Laplace Equation

Starting with Fick's Second Law

Fick's second law describes how the concentration of a diffusing substance changes over time. It is given by:



Where:

* C is the concentration of the diffusing substance,
* 𝑡t is time,
* 𝐷 is the diffusion coefficient, and
* ∇2 is the Laplacian operator.

Steady-State Condition

In steady-state diffusion, the concentration does not change over time, so the time derivative term  ​ vanishes:



Substituting into Fick's Second Law

When we substitute  into Fick's second law, we get:



This equation represents the steady-state diffusion process, where the Laplacian of the concentration  is equal to zero.

General Form of the Laplace Equation

The resulting equation,  is known as the Laplace equation. It is a second-order partial differential equation that describes systems in which the quantity of interest (in this case, concentration) is in a state of equilibrium, with no sources or sinks.

Extending to Two Dimensions

When considering diffusion in two dimensions, we extend the Laplace equation by adding derivatives with respect to the additional spatial dimensions (e.g., *x* and *y*). This yields the 2D Laplace equation:



This equation describes the steady-state distribution of concentration in a two-dimensional space.

Solving The Equation With SOR

The Successive Over-Relaxation (SOR) method is an iterative technique used to solve linear systems of equations, particularly those arising from discretized partial differential equations like the Laplace equation. It is an extension of the Gauss-Seidel method, incorporating a relaxation parameter to accelerate convergence.

Initialization:

Choose an initial guess for the concentration C at each grid point. Set the relaxation parameter ω (typically between 1 and 2) and choose a convergence tolerance. (ω =1.9 is the best for most case)

Iteration:

Iterate through each grid point, excluding the boundary points. Update the concentration value at each grid point using the SOR formula:



where:

*  is the concentration at grid point (𝑖,𝑗)in the 𝑘-th iteration.
*  and  are the concentrations at the neighboring grid points.
* *ω* is the relaxation parameter.

Convergence Check:

Compute the change in concentration values between the current and previous iterations. Check if the maximum change falls below the specified tolerance level. If so, stop iterating; otherwise, continue.

Solution Extraction:

After convergence is achieved, the concentration values at each grid point represent the numerical solution to the Laplace equation.

Conclusion**:**

Through the meticulous application of the SOR method, the Laplace equation governing steady-state diffusion can be effectively solved, offering valuable insights into concentration dynamics within the system. This iterative approach not only facilitates computational efficiency but also enhances the understanding of diffusive phenomena in diverse scientific and engineering contexts.

References:

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# “Successive over-relaxation method” – ESE Jupyter Material:

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