

Device Simulation Laboratory

(EE5195)

Problem Sheet-7

Q.1: Numerical solution of Time dependent Diffusion equation

(a) Describe the formalism to solve time dependent diffusion equation using backward Euler scheme.

(b) Consider a region of length $10\text{ }\mu\text{m}$. Assume perfectly absorbing boundary conditions at $x=0$ and at $x=10\text{ }\mu\text{m}$. At time $t=0$, assume that particles are injected at $x=5\text{ }\mu\text{m}$ is such that the density is 10^6 cm^{-3} (i.e., the injection is a delta function in both space and time). Using the formalism described in (a) explore the evolution of particle density over the specified domain (use $D=10^{-4}\text{ cm}^2/\text{s}$). Compare with analytical results. Explore the significance of the parameter.

Q.2: Random Walk simulations:

(a) Discretize the time dependent diffusion equation and arrive at a scheme for solving the time dependent diffusion equation through random walk simulations. For $D=10^{-4}\text{ cm}^2/\text{s}$ and $\Delta x=10\text{ nm}$, what should be the Δt , the time step in such simulations?

(b) Assume that $N=100$ particles are released at $x=5\text{ }\mu\text{m}$ at $t=0$. Explore the evolution of particle density profile as a function of time using random walk simulations. Compare with analytical results. Explore the density function for $N=1000$, and $N=10000$ particles.