Project 13 PDE MOLECULAR DIFFUSION OF ALCOHOL VAPORS IN A TUBE

1. INTRODUCTION TO THE PROBLEM

In this problem we consider the physical phenomenon of the diffusion of alcohol vapor molecules present in quantities equal to 2% of the total air inside a tube of 20cm length.
At the bottom of the tube there is a tray of alcohol which evaporates into the stagnant gas above. (The external environment provides heat by keeping the alcohol at a constant temperature of 30°C, at which the vapor pressure is equal to 0.1 atm).
At the upper end of the tube, the vapors are dispersed in the outside air so that the concentration u is essentially equal to zero.
Before moving on to the description of the mathematical model it is therefore necessary to understand what is meant by molecular diffusion.
Diffusion is the phenomenon whereby the molecules of a solution naturally tend to pass from the areas with a higher concentration to those with a lower concentration. When two different substances are mixed, the molecules of both diffuse until they reach an equilibrium concentration. The different diffusion phenomena follow the same laws, valid, with good approximation, in most of the real cases. The diffusion rate is proportional to the concentration, temperature or charge gradient (when the gradient is small). The diffusion speed depends on specific properties of the diffusing material, through a parameter which, in the case of heat or electricity, is called conductivity, while in the case of matter it is called the diffusion coefficient. Since, according to the laws of thermodynamics, every system tends to reach the condition of equilibrium, the molecules that are in a zone with greater concentration tend spontaneously to move towards the zone in which they are less concentrated; in other words, they are said to move "according to concentration gradient". Inside a container full of water, for example, the particles of a drop of ink tend to move away from each other and arrange themselves evenly in the liquid that contains them (diffusion phenomenon). If we consider two solutions having different concentrations and separated by a semipermeable membrane, that is, which allows only the passage of the solvent molecules and not the solute, the solvent flows towards the more concentrated solution, in which there are more particles of solute and less than solvent (osmosis phenomenon).

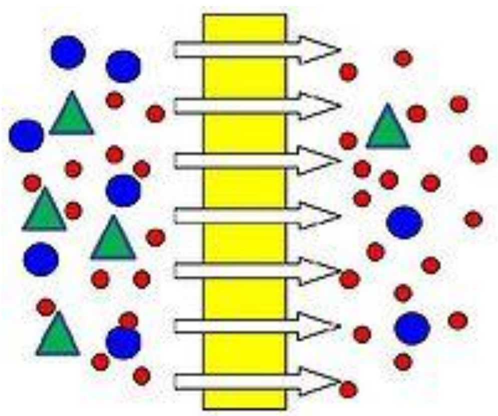

Fig.1 –diffusion-

DESCRIPTION OF THE MATHEMATICAL MODEL

In particular, the problem under consideration is governed by the diffusion equation set according to the Cauchy problem:

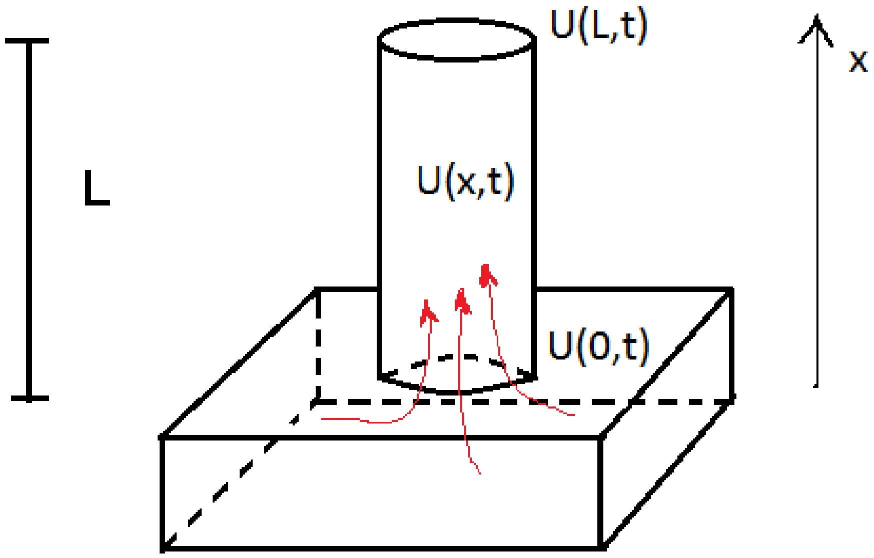

Fig. 2 –physical model-

$$
\begin{cases}
\delta u/\delta t = a^2 \delta^2 u/\delta x^2; & 0 < x < L,\ t > 0 \\
u(x,0) = 2.0; & 0 \le x \le L \\
u(0,t) = 0, u(20,t) = 10; & t > 0
\end{cases}
$$

The equation is accompanied by an initial data and boundary conditions (or Dirichlet), which represent situations in which the concentration at the boundary of the domain has a known a priori trend.

Here a^2 = 0.119 cm^2/sec is the diffusion coefficient.

It is required to numerically integrate the above problem using and comparing the following finite difference schemes:

1) Euler methods (explicit and implicit)
2) Crank-Nicolson method.