CHAPTER I

INTRODUCTION

One of the problems often encountered by the chemical engineer is to find the transient temperature distribution in a solid where the initial temperature distribution is known and the boundary conditions are specified. This involves finding either the exact solution to the governing partial differential equation, commonly called the diffusion equation, or obtaining a reasonably accurate estimate of its solution for the specific conditions of the problem. To obtain the transient temperature distribution numerically, using either a known exact solution or an approximate method, usually requires a great many tedious, time-consuming calculations. Since most problems of engineering importance are too complicated for analytic solution, an approximation is necessary. Even when the exact solution is available (1), or can be found, it often requires more calculations to find the numerical solution than does an approximate calculation. Therefore, as an engineer is interested in finding a numerical solution that is sufficiently accurate for his purposes with a minimum of effort, an approximate method can be a practical and economical tool for him to use.

This study is on approximate methods of finding numerical solutions to the diffusion equation that can be applied to a wide range of problems, that are of reasonable accuracy, and that are relatively easy to use. Although many of the methods discussed here require a high-speed computer, for problems in one space dimension a graphical method is shown analytically to give reasonably accurate results. If a desk calculator is available, further significant improvements can be made without the cost in time and money of programming and running a digital computer. The methods that require a high-speed computer are for a very general problem and, in contrast to most methods, are based on a relatively coarse difference grid. In all cases, particular emphasis is placed on problems where the boundary conditions involve a finite heat-transfer coefficient.

For chemical engineers the diffusion equation is probably the most important partial differential equation. In addition to governing the transient temperature distributions in solids, it, or a closely related equation, governs certain situations in diffusional mass transport, fluid mechanics, and energy transfers in fluid systems. Although this study is concerned only with the linear diffusion equation without sources or sinks (equation II-4), generalizations to many of the related equations are possible.

To use an approximate numerical method, the derivatives are replaced with differences for a finite number of points within and on

the solid boundary. This approximation, together with similarly approximated boundary conditions, gives either a linear system of ordinary differential equations or a system of algebraic equations to be solved to determine the transient temperature distribution. The system of ordinary differential equations can be solved almost instantaneously with an electric analog computer; the algebraic equations can be solved rapidly for successive time increments on a digital computer. Complicated initial temperature distributions and/or complicated boundary conditions for which it is impossible to find the exact solution are usually easily handled by the approximate method.

The advent of the high-speed digital computer, because of its capability of carrying out an enormous amount of calculations in an extremely short time, has made practical many of the classical methods of approximation and has greatly stimulated studies of difference methods for obtaining approximate numerical solutions to the diffusion equation. Starting in 1950, several important articles about the approximate methods for solving the diffusion equation have been published. O'Brien et al. (2) showed, both by theoretical arguments using a method of von Neumann, and by a numerical check, that the unstable behavior of certain approximations to the diffusion equation is a property of the difference scheme used and is not caused, but can be aggravated, by round-off error. In 1956 Lax and Richtmyer (3) showed that, for a wide range of linear initial-value problems including the diffusion equation,

in principle the approximate solutions can be made as accurate as desired, by using smaller and smaller difference increments, if the approximate solution remains stable and if the approximation is "consistent."

Since 1955, results from matrix algebra have been used to attack the stability problems by Todd (4) and Franklin (5), and accuracy problems by Varga (6,7). In addition, numerous other articles have appeared and many reviews of approximate methods for the diffusion equations are found in recent texts. Most of these articles and discussions are concerned with problems where the geometry is such that it may be represented by temperature points located in a regular, repeated geometric pattern, and where the boundary conditions are either a specified surface temperature (infinite heat-transfer coefficient) or adiabatic (zero heat-transfer coefficient). The important published results can be discussed more appropriately in sufficient detail later.

The two major goals of this research have been (1) to devise a reasonably accurate approximate method for calculating transient temperature distributions in solids with irregular boundaries without using an extremely fine space grid; and (2) to develop good methods of approximating the boundary condition equations for the practical case of finite heat-transfer coefficient.

The first problem has been studied by MacNeal (8), who suggested using an asymmetric location of the temperature points so that they

could be located on the irregular boundary. He also presented a set of rules for approximating the Laplacian operator. Longwell (9) has adapted this scheme to an explicit method for stepping out the transient temperature distribution. The asymmetric location of temperature points as applied to the transient problem raises two difficulties. First, since the points are not located regularly, the usual methods of finding stability criteria do not work. Second, errors are introduced by asymmetric location of the points. For example, 20,000 to 100,000 points have been used (6) for the steady-state solution in two dimensions. This shows the practical importance of obtaining a good approximation for the Laplacian which does not require an extremely fine space grid for irregular solids. Using a grid with this number of points is impractical or uneconomic for the transient problem. Moreover, for problems in three space dimensions or for a simulation problem where the transient temperature calculation is only a small part of the total problem, a good approximation using a coarse grid would be very desirable.

The most realistic boundary conditions for solids are those which have a finite heat-transfer coefficient. In spite of this, essentially no theoretical studies have been made of good methods to approximate this "third" (10) boundary condition. There are few practical discussions of this type of boundary condition.

The next chapter contains mostly introductory material upon which the following chapters are based. The problem of transient

temperature distribution is formulated as the solution to the partial differential equation of diffusion with its initial and boundary conditions. The MacNeal-Longwell (9) method is used to formulate the approximate equations. The analytic solutions are shown in symbolic form for both formulations. The emphasis is on pointing out the many similarities between the continuous and the approximate formulations. These similarities are in the derivations of both the continuous and approximate equations, in the form of their solutions, and in properties of the continuous and difference operators.

Chapter III presents the stability criteria for an approximate solution based on a network of points located either regularly or irregularly. An example problem for transient heat transfer in two space dimensions is also shown to check these results. This problem shows that an asymmetric point distribution does give a reasonably accurate solution. In Chapter IV the accuracy of approximations based on uniform mesh spacing for a problem in one space dimension in Cartesian coordinates is discussed in detail. To do this a z-transform method is developed for the solution of the partial difference equation of diffusion. Several methods for the approximation for boundary conditions with finite heat-transfer coefficients are presented. The accuracy of these methods is compared analytically for both generalized methods and graphical methods. Chapter V gives a detailed discussion of errors introduced by the asymmetric distribution of points for problems in two

space dimensions, and gives a general set of rules for location of the points.

Before starting the actual study several general comments should be made about the nomenclature. Although every effort has been made to try not to use the same symbol in two ways; to have a representation for matrices, vectors, and scalars; and yet to use standard chemical engineering nomenclature; many conflicts can and do occur. Capital Roman letters are generally used to represent matrices, small Roman letters to represent vectors, and Greek letters for scalars. Sometimes in the sequence of matrices, vectors, and scalars, when this has not been possible, an element of a matrix or a vector may be designated with a small Roman letter with a double or single subscript, respectively.

The main exception to the sequence of capital and small Roman letters, and Greek letters, is that standard chemical engineering nomenclature has been maintained, which gives rise to some inconsistencies. Also, in matrices, i refers to the row and j to the column. The subscripts i and m are used to designate temperature points, the distinction being that m refers to a uniform network so that its numerical value has a physical meaning. The letter T is used for the exact continuous solution of the partial differential equation and t for an approximate solution. The two letters represent vectors evaluated at a time if they are shown, $T(\tau)$ and t_n with elements $T_i(\tau)$ and

$t_{i,n}$. In using these symbols, the first subscript indicates an increment of space and the second time an increment of time; if only one is used, the quantity represents a vector at the time corresponding to the subscript. In cases where ambiguity may result, the quantity is defined in the text before or just after its first use.

Several comments may also add to the clarity of the text. The formulation and solution of the partial differential equation are referred to as the continuous formulation and solution. The difference or analog solutions to the continuous problem are referred to as approximate solutions. Since numerical results may be obtained from either the continuous or approximate formulation, the terms "numerical method" and "numerical solution" have been avoided. "Similar" is used in its precise mathematical meanings, that is, similar matrices have the same eigenvalues, and similar nodes are those that have the same angles and proportionate lengths.