CHAPTER II
BACKGROUND AND LITERATURE SURVEY

There are many applications of mathematical methods in various fields of study. This work is focused on representative problems in chemical engineering, which are analyzed by finite element method. Development of this including finite element method is as follows:

2.1 Finite Element Procedure

Although the finite element procedure depends on an individual user, the implementation of the finite element approach usually follows a six standard step, (Dechaumphai, 1998):

2.1.1 <u>Discretization</u>

This step involves dividing the problem domain (geometry) into a finite number of small subregions called "elements". Many convenient shapes are available, such as triangles and quadrilaterals in two dimensions, and tetrahedral, pentrahedral, and hexahedral for three dimensions. The points of intersection of the lines that make up the sides of the elements are referred to as "node". Figure 2.1 shows an example of system discretization of system into finite elements.

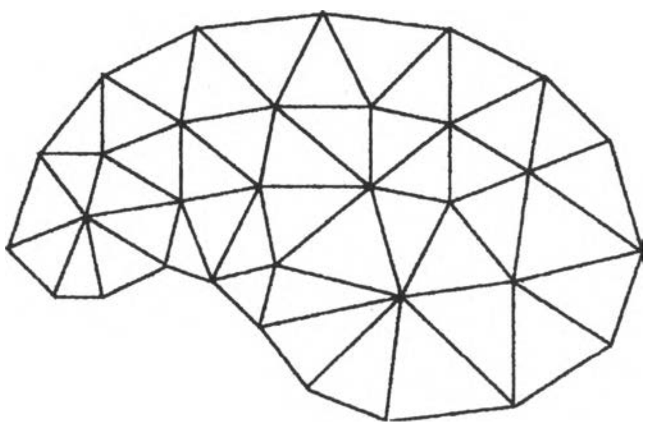

Figure 2.1 The discretization of a system into finite elements.

2.1.2 Solution Form

To approximate solution, a solution form will be built by choosing an appropriate function, which is a relatively simple function, with unknown coefficients. For example, for one-dimensional problem, the simplest alternative form is a first order polynomial,

$$u \approx v(x) = a_0 + a_1 x \qquad (2.1)$$

where u(x) is a dependent variable, a_0 and a_1 are unknown constants, and x is an independent variable. The higher order of polynomial was proved to give more accurate solution. The solution then can be rewritten as,

$$v(x) = \gamma_1 v_1 + \gamma_2 v_2 \qquad (2.2)$$

where γ_1 and γ_2 are called "interpolation functions", and v_1 and v_2 represent dependent variables at node 1 and 2 in the element. It can also be exhibited in an equivalent matrix form,

$$v(x) = \begin{bmatrix} \gamma_1 & \gamma_2 \end{bmatrix} \begin{Bmatrix} v_1 \\ v_2 \end{Bmatrix}. \qquad (2.3)$$

2.1.3 Element Equation

This step is considerably a heart of the finite element method. Once the interpolation function is chosen, the equation governing the behavior of the system must be developed. This equation represents a fit of function to solution of the underlying differential equation. Several methods are available for this purpose. Among the most common methods are the direct approach, the method of weighted residuals, and the variation approach. These methods will specify relationships between the unknowns in equation (2.2) that satisfy the underlying partial differential equation in an optimal fashion.

Mathematically, the resulting element equations will often consist of a set of linear algebraic equations that can be expressed in a matrix form,

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{Bmatrix} v_1 \\ v_2 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \end{Bmatrix}, \text{ or} \quad (2.4)$$

$$Av = b. \quad (2.5)$$

where coefficient matrix A is an "element property or stiffness matrix", v is a column vector of unknowns at nodes, and b is a column vector reflecting the effect of any external influences applied at the nodes.

2.1.4 Assembly

After the individual element equations are derived, they must be linked together or assembled to characterize the unified behavior of the entire system. The enlarge matrix, or system matrix, will be in form of band matrix, which allows simplification to be made in implementation step.

2.1.5 Boundary Conditions

This step is to apply boundary condition into the system equation. These adjustments result in a system matrix, which is ready to be solved.

2.1.6 Solution

Solution of equation prepared in 2.1.5 can be obtained with conventional techniques that generally are used for solving system of linear algebraic equations e.g., iteration or Gauss elimination methods.

2.2 The Development of Finite Element Method

The finite element method has been originally introduced and early used by engineers to analyze aircraft structural systems using the emerging scientific digital computer (Baker and Pepper, 1991). The most important reason for its development existed from the desire to solve difficult problems from structural mechanics in a relatively simple way. From the viewpoint of simplicity of formulation, it is surprising that the method has been developed for structural analysis, because the application to the solution of many other partial differential equations is definitely easier to perform. However, application of the finite element method to non-structural problems was first reported by Zienkiewicz and Cheung (1965). Since then, there have been many contributions and developments of mathematical theory of finite elements, which objected to deal with higher and higher complicate problems. The concept of finite element is now spreading globally to solve a great number of problems in various fields of study. For example, Janphaisaeng (1998) analyzed system of high speed compressible flow via finite element method, Liu and Reitz, (1998) used FEM to model heat conduction in chamber walls in engine simulation and Caire *et al.* (2001) used the concept for modeling fluorine electrolyzer.

2.3 Finite Element Method with Poisson's Equation

Poisson's equation is very useful to describe the state of heat conduction and mass diffusion, which are important phenomena in chemical engineering. It also gives advantage coupling with stream or potential function concept. Here, emphasizing in the present work, its finite element properties were discussed.

Haroutian and Betts (1983) showed the capability of finite element solution with a stream function by applying with two-dimensional natural convection.

Fletcher (1983) compared finite element and finite difference methods in computational fluid dynamics on the basis of convergence properties, accuracy, economy and computational efficiency. The results stated that when the maximum time-step used was limited by stability, the higher order schemes generally produce higher accuracy. The quadratic finite element and five-point finite difference schemes appear to be the most efficient. Increasing the order of a finite element scheme in more than one dimension produces a much less economical computation than increasing the order of a finite difference scheme. This effect is worse in three than in two dimensions.

2.4 Partial Differential Equation Solver

With high complexity of various kinds of PDE problems, several solutions have been proposed. Computational approach inevitably plays an extremely important role to deal with such problems.

Machura and Sweet (1980) surveyed softwares for partial differential equations and proposed classification of them. Based upon the automation level achieved, PDE software tools were classified into five classes,

(a) a program solving a given PDE problem
(b) a program package with a standard programming language interface
(c) a program package with a special language interface
(d) a special-purpose language with no direct reference to PDEs
(e) an extension of a standard programming language by including finite-difference operators.

Here, closest to the present work, the first class was focused. Programs of this kind are of great practical importance. They very often handle the most challenging real-life PDE problems. The usefulness of these programs is frequently measured by the speed and memory requirements. It is not surprising to find that such special-purpose programs are mainly used as production software in many branches of industry.