CHAPTER III
PROBLEM SOLVING METHOD

3.1 Differential Equation

Differential equations selected to study in this work are in the class of "Poisson's Equation", which has a general form of

$$\nabla u \cdot k\nabla u + f - gu = 0, \tag{3.1}$$

and its related transient form of

$$\nabla u \cdot k\nabla u + f = g\frac{\partial u}{\partial t}. \tag{3.2}$$

These kinds of equation cover many problems, especially, in the engineering modeling. For example, in chemical engineering field, they will be used to deal with the problems of heat conduction, mass diffusion analysis, etc. Here, practical three types of boundary condition were supplemented. Those are as follow:

1. Dirichlet Boundary Condition. The surface covering this boundary type is represented as S1, with a constant dependent variable on this surface.

$$u = u(\text{specific}). \tag{3.3}$$

2. Neumann Boundary Condition. The surface covering this boundary type is represented as S2. On this surface, flux normal to surface is zero. That is

$$k\frac{\partial u}{\partial n} = 0. \tag{3.4}$$

3. Mixed Boundary Condition. This type is known as S3 type boundary, which has a general form of

$$k\frac{\partial u}{\partial n} + \alpha u = \beta . \tag{3.5}$$

3.2 Finite Element Analysis of Poisson's Equation

3.2.1 Galerkin Residual Equation

From governing equation in 3.1, the corresponding finite element equation was developed. Supposed the basis function as

$$u \approx v = \sum_{j=1}^{m} \gamma_j v_j . \tag{3.6}$$

For linear triangular elements, all basis functions would be zero except those corresponding to three vertices p, q and r and would be reduced to

$$v = \gamma_p v_p + \gamma_q v_q + \gamma_r v_r . \tag{3.7}$$

In the first step, Galerkin statement was applied to Poisson's equation,

$$\int_V \gamma_i (\nabla \cdot k\nabla u + f - gu) dV = 0 . \tag{3.8}$$

Then, apply Green's theorem (Shown in Appendix A) to the first term gives,

$$\int_V \gamma_i \nabla \cdot k\nabla u dV = -\int_V k\nabla\gamma_i \cdot \nabla u dV + \int_S \gamma_i k\frac{\partial u}{\partial n} dS . \tag{3.9}$$

Back substitution hence,

$$\int_V k\nabla\gamma_i \cdot \nabla u dV + \int_V \gamma_i g u dV = \int_V \gamma_i f dV + \int_S \gamma_i k\frac{\partial u}{\partial n} dS \tag{3.10}$$

Incorporating the trial function (Equation 3.6) yields,

$$\int_V k\nabla\gamma_i \cdot \sum_{j=1}^{m}(\nabla\gamma_j)v_j dV + \int_V g\gamma_i \sum_{j=1}^{m}\gamma_j v_j dV = \int_V \gamma_i f dV + \int_S \gamma_i k\frac{\partial u}{\partial n} dS \qquad (3.11)$$

The surface integral (last term in Equation 3.11) depends on what type of boundary that surface cover, and have value of following individually

1. S1 - type, since points i = 1, 2, 3, ... , n have been arranged not coincide with S1 boundary. So that, $\gamma_i = 0$ on S1 and surface integral is therefore zero.
2. S2 - type, since $k\frac{\partial u}{\partial n}$ equal to zero, thus, its integral equal to zero.
3. S3 - type, inserting (3.5) into surface integral term gives

$$\int_{S3} \gamma_i \left(\beta - \alpha \sum_{j=1}^{m} \gamma_j v_j \right) dS .$$

So, a more general form of Equation 3.11 can be written as

$$\int_V k\nabla\gamma_i \cdot \sum_{j=1}^{m}(\nabla\gamma_j)v_j dV + \int_V g\gamma_i \sum_{j=i}^{m}\gamma_j v_j dV + \int_{S3} \alpha\gamma_i \sum_{j=1}^{m}\gamma_j v_j dS = \int_V \gamma_i f dV + \int_{S3} \beta\gamma_i dS , \qquad (3.12)$$

which is ready to cooperate S3 type boundary condition. Equation 3.12 can be represented in a matrix form of Av = b, where each element of coefficient matrix A and vector b are defined as

$$a_{ij} = \int_V k\nabla\gamma_i \cdot \nabla\gamma_j dV + \int_V g\gamma_i\gamma_j dV + \int_{S3} \alpha\gamma_i\gamma_j dS , \qquad (3.13)$$

$$b_j = \int_V \gamma_i f dV + \int_{S3} \beta\gamma_i dS - \sum_{j=1}^{m} a_{ij} v_j , \qquad (3.14)$$

3.2.2 Linear Triangular Elements and Basis Functions

Starting with rectangular coordinate; consider triangular element shown in Figure 3.1

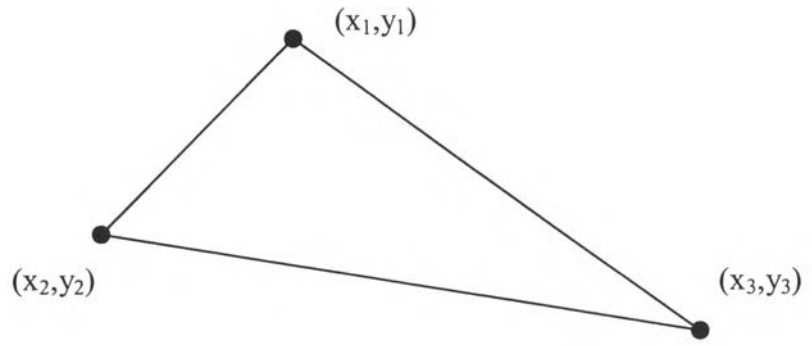

Figure 3.1 Triangular element

Inside the triangle element, a dependent variable v is assumed to be a linear function of position. Analogy to Equation 3.7, it is a linear combination of three nodal values v_1, v_2 and v_3 as

$$v = a + bx + cy = \gamma_1 v_1 + \gamma_2 v_2 + \gamma_3 v_3 , \tag{3.15}$$

where basis functions γ_1, γ_2 and γ_3 vary linearly with position as,

$$\gamma_i = \frac{1}{2\Delta}(a_i + b_i x + c_i y) \tag{3.16}$$

where Δ is the area of element given by the determinant:

$$\Delta = \frac{1}{2}\begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = \frac{1}{2}(a_1 + a_2 + a_3) \tag{3.17}$$

Nine coefficients, a_i, b_i, c_i, (i = 1, 2, 3) can be deduced by requiring that each basis function γ_i is one at node i and zero at other two nodes. After some manipulations, the results are:

$$
\begin{aligned}
a_1 &= x_2y_3 - x_3y_2 & a_2 &= x_3y_1 - x_1y_3 & a_3 &= x_1y_2 - x_2y_1 \\
b_1 &= y_2 - y_3 & b_2 &= y_3 - y_1 & b_3 &= y_1 - y_2 \\
c_1 &= x_3 - x_2 & c_2 &= x_1 - x_3 & c_3 &= x_2 - x_1
\end{aligned}
\tag{3.18}
$$

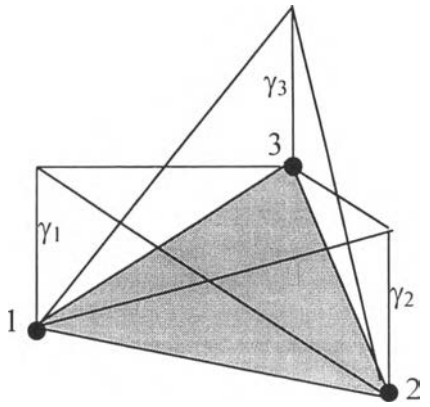

Figure 3.2 Three basis functions with each $\gamma_i = 1$ at node i, declining linearly to zero at other two nodes.

Table 3.1 shows integration formulas involving linear basis functions. The results for integration over a triangular element are derived from the general formula:

$$\int_{\Delta} \gamma_1^q \gamma_2^r \gamma_3^s d\Delta = \frac{q!r!s!}{(q - r + s + 2)!} 2\Delta \tag{3.19}$$

To solve the equation regional integrals, summation of the contributions from the individual elements must be obtained.

$$\int_V g\gamma_i\gamma_j dV = \sum_{e=1}^{n_e} \int_{\Delta_e} g^e \gamma_i^e \gamma_j^e d\Delta^e \,, \tag{3.20}$$

where n = number of element and superscript e denote values associated with element e. After coefficient matrix A and vector b was built, simultaneous linear equation will be solved. The surface flux next will be determined.

Table 3.1 Integration formulas involving linear basis functions, for triangular elements and line boundary segments.

Area Integrals		Line Integrals	
Integral	Value	Integral	Value
$\int \gamma_i d\Delta$	$\frac{1}{3}\Delta$	$\int \gamma_i dL$	$\frac{1}{2}L$
$\int \gamma_i^2 d\Delta$	$\frac{1}{6}\Delta$	$\int \gamma_i^2 dL$	$\frac{1}{3}L$
$\int \gamma_i \gamma_j d\Delta$	$\frac{1}{12}\Delta$	$\int \gamma_i \gamma_j dL$	$\frac{1}{6}L$
$\int \gamma_i^3 d\Delta$	$\frac{1}{10}\Delta$	$\int \gamma_i^3 dL$	$\frac{1}{4}L$
$\int \gamma_i^2 \gamma_j d\Delta$	$\frac{1}{30}\Delta$	$\int \gamma_i^2 \gamma_j dL$	$\frac{1}{12}L$
$\int \gamma_i \gamma_j \gamma_k d\Delta$	$\frac{1}{60}\Delta$		

3.2.3 Solution of Poisson's Equation in Cylindrical Coordinates

For axisymmetric cylindrical coordinates, dV and dS are equal to 2π rdrdz, and 2πrdL respectively. The elements of coefficient matrix and vector b change to,

$$a_{ij} = \int_V \left(\frac{\partial \gamma_i}{\partial r}\frac{\partial \gamma_j}{\partial r} + \frac{\partial \gamma_i}{\partial z}\frac{\partial \gamma_j}{\partial z} \right) r dr dz + \int_V g\gamma_i\gamma_j r dr dz + \int_{S3} \alpha\gamma_i\gamma_j r dL, \qquad (3.21)$$

$$b_j = \int_V \gamma_i f r dr dz + \int_{S3} \beta\gamma_i r dL - \sum_{j=1}^{m} a_{ij} v_j . \qquad (3.22)$$

To evaluate new integrals, consider r as a combination of three vertex values (r_i, r_p and r_q)

$$r = \gamma_i r_i + \gamma_p r_p + \gamma_q r_q \tag{3.23}$$

Consider a representative term in a_{ij}

$$I = \int_{\Delta_e} g\gamma_i\gamma_j r dr dz = \int_{\Delta_e} g\gamma_i\gamma_j\left(\gamma_i r_i + \gamma_p r_p + \gamma_q r_q\right) d\Delta^e \tag{3.24}$$

Suppose $i \neq j = p$, The Integration in Equation 3.24 will be

$$I = g^e\Delta^e\left(\frac{1}{30}r_i + \frac{1}{30}r_j + \frac{1}{60}r_q\right) = \frac{1}{12}g^e\Delta^e\left(\frac{1}{5}r_i + \frac{1}{5}r_j + \frac{3}{5}\bar{r}\right) \tag{3.25}$$

in which $\bar{r} = \left(r_i + r_p + r_q\right)/3$ is the radius of the element centroid. If i = j, Equation 3.24 becomes

$$I = \frac{1}{6}g^e\Delta^e\left(\frac{2}{5}r_i + \frac{3}{5}\bar{r}\right) = \frac{1}{6}g^e\Delta^e\left(\frac{1}{5}r_i + \frac{1}{5}r_j + \frac{3}{5}\bar{r}\right). \tag{3.26}$$

Table 3.2 shows multiplying factors for obtaining element contributions in r/z coordinates from those in x/y coordinates.

Table 3.2 Multiplying factors for obtaining element contributions in r/z coordinates from those in x/y coordinates.

Integral	Factor
$\int_v k\nabla\gamma_i \cdot \nabla\gamma_j r dr dz$	$\bar{r}$
$\int_v g\gamma_i\gamma_j r dr dz$	$\frac{1}{5}\left(r_i + r_j + 3\bar{r}\right)$
$\int_{s_j} \gamma_i\gamma_j r dL$	$i = j: \frac{1}{2}\left(r_i + \bar{r}\right)$ $i \neq j: \bar{r}$
$\int_v \gamma_i f r dr dz$	$\frac{1}{4}\left(r_i + 3\bar{r}\right)$
$\int_{s_j} \beta\gamma_i r dL$	$\frac{1}{3}\left(r_i + 2\bar{r}\right)$

3.2.4 Initial Value Problem

In the previous section, the Poisson's equation was treated whose finite element formulation was,

$$Av = (K + G)v = b. \tag{3.27}$$

Matrix K includes the contributions from the conductive ($\nabla k \nabla u$) and the mixed (S_3) type boundary conditions. Matrix G contains the variable part (- gu) of the source term. Vector b incorporates terms derived from both the constant part (f) of the source term and a surface integral arising from application of Green formula.

Here, related form of time-dependent problem will be considered. The equation will be in the form of,

$$\nabla \cdot k\nabla u + f = g\frac{\partial u}{\partial t}. \tag{3.28}$$

By analogy to Equation 3.27, the finite element solution of Equation 3.28 should be in the form of,

$$Kv + G\frac{dv}{dt} = b \tag{3.29}$$

where K, G and b are as already formulated, and v is now a time-dependent vector of nodal solution. Now, the finite difference method is cooperated to solve such equation. Here, superscript n denotes values at time t and n + 1 mean values at time t + Δt, and Crank-Nicolson method is applied,

$$K\frac{\left(v^n + v^{n+1}\right)}{2} + G\frac{\left(v^{n+1} - v^n\right)}{\Delta t} = \frac{1}{2}\left(b^n + b^{n+1}\right) \tag{3.30}$$

Define new terms,

$$R = \frac{1}{\Delta t}G + \frac{1}{2}K, \qquad S = \frac{1}{\Delta t}G - \frac{1}{2}K. \tag{3.31}$$

System of linear equations can be obtained as,

$$Rv^{n+1} = Sv^{n} + \frac{1}{2}\left(b^{n} + b^{n+1}\right), \tag{3.32}$$

and new solution at time t + Δt is,

$$v^{n+1} = R^{-1}Sv^{n} + \frac{1}{2}R^{-1}\left(b^{n} + b^{n+1}\right) \tag{3.33}$$

3.3 Programming Strategy

3.3.1 Program Description

Corresponding to the finite element equation created in 3.2, a new application program named "**FEM**" was built via Visual Basic 6.0 (based upon the program by Wilkes, 1995). The developed program consists of six work forms, and two more separated modules, and 46 subprograms (or event procedures). All forms, modules, and subprograms are shown in Table 3.3. However, details of interface and source code for each form or module are shown in appendix B through C.

Table 3.3 All forms, modules, and subprograms in "FEM"

Form or Module	Subprogram or procedure
FrmAbout	**Event Procedure** • Form_Load() • CmdOK_Click()
FrmFemwork	**Subprogram** • DataInput() • DataShow() • Draw_mesh() **Event Procedure** • CmdBack_Click() • CmdForm_Load() • CmdSolve_Click()
FrmInput	**Event Procedure** • CmdBrowse_Click() • OptCreate_click() • OptImport_click() • CmdOK_Click()
FrmMain	**Subprogram** • LoadNewWork() **Event Procedure** • MDIForm_Load() • MDIForm_Unload() • MnuEditCopy_Click() • MnuEditCut_Click() • MnuEditPaste_Click() • MnuFileExit_Click() • MnuFileNew_Click()

Form or Module	Subprogram or procedure
	• MnuAboutAbout_Click() • TbToolBar_ButtonClick()
FrmResult	**Subprogram** • DrawBoundary() • DrawContU() • DrawMesh() • PrepareData() • ReportData() • ShowSol() **Event Procedure** • CmdClear_Click() • CmdContU_Click() • CmdMesh_Click() • CmdSetPara_Click() • CmdSimul_Click() • Form_Load() • TmeClocl_Tmier()
FrmSetPara	**Event Procedure** • CmdDefault_Click() • CmdOK_Click()
Calculation (Module)	**Subprogram** • Asembl() • Fluxes() • Gelb() • Geom() • MainProg()

Form or Module	Subprogram or procedure
	• Matrix() • NewVal() • PrtSol()
Complementation (Module)	**Subprogram** • Main()

3.3.2 Calculation Procedure

The calculation procedure consists of four steps as shown below,

3.3.2.1 Input Data

This step is to read all required data for a particular problem, consisting of general system data, element, nodal, and boundary conditions information, from specific data file. This step is in the subprogram "InputData" in form "frmInput". Next step, the subprogram "MainProg" in module "Calculation" is called. The calculation starts here.

3.3.2.2 Form Element and System Equation

This step is to create finite element matrix for each element in the subprogram "Geom" and "Matrix". Then, they are assembled together to form the system matrix and supplemented S3 boundary condition simultaneously by the subprogram "Asembl".

3.3.2.3 Solution

Consequently, the system equation is solved in the subprogram "NewVal" by using Gauss Elimination Method with column pivoting in the subprogram "Gelb".

3.3.2.4 Result Exhibition

In this step, the numerical result obtained from 3.3.2.3 is exhibited in a table in the form "frmResult". Graphical result is also exhibited by the choice of user, including showing meshing, constant lines of dependent variable, or simulation (case of transient problem).

Coarse flow diagram showing all calculation steps is shown in Figure 3.3.

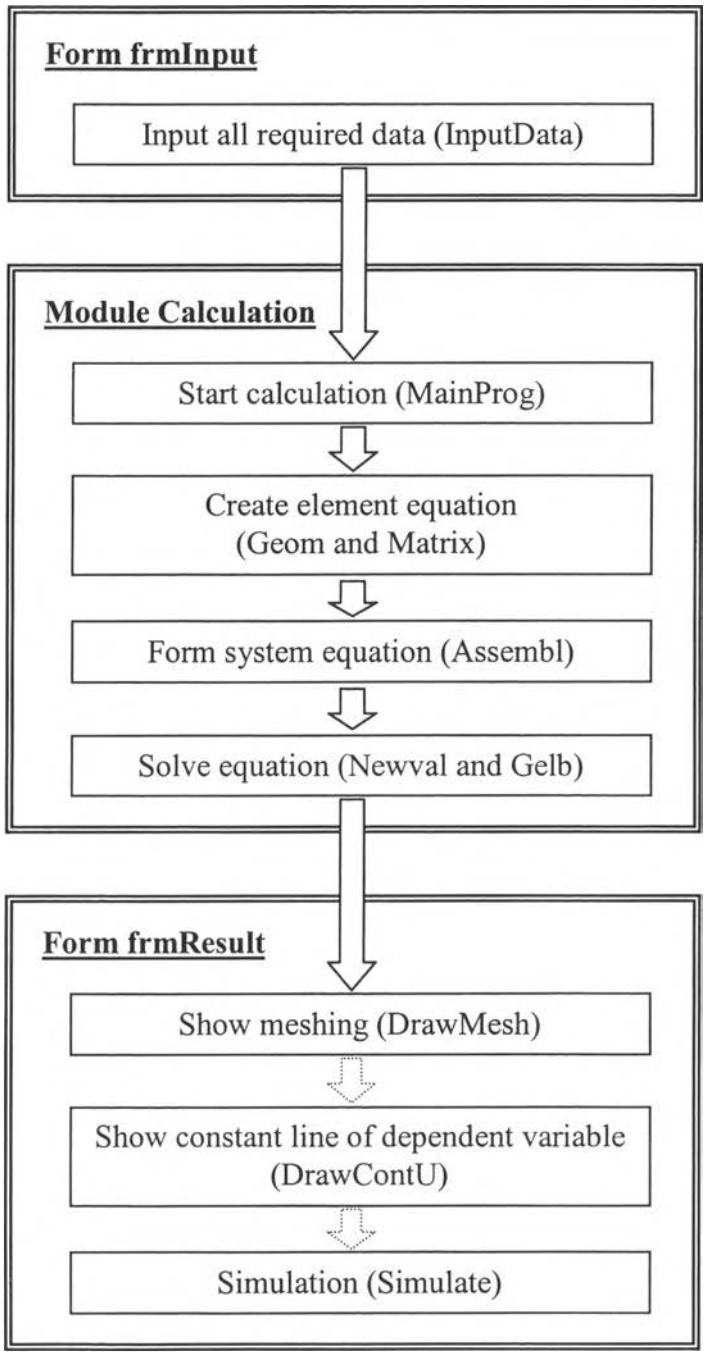

Figure 3.3 Coarse flow diagram of program "FEM"

3.3.3 Data Input File Format

The data file for supplement into the program is in a simple text file format, which can easily be created by any text editors such as "notepad" or "wordpad". The data file requires four parts including general system data, element, nodal and boundary condition information respectively. These are details of each part.

Part I General System Data

This part contains problem name, coordinate system, error tolerance, variation of K, F, and G, steady or unsteady state parameter, variation of S1 and S3 type boundary condition parameters, element type, number of elements, nodes, and boundary segments. All these data are in a line series starting from first column for each line. The example is represented here. Data in line number 12-14 is optional for transient problems. The value of individual parameter is found through Appendix C.

Example

```
Line  data
1     TRANSIENT HEAT CONDUCTION IN SLAB
2     ALL PARAMETERS:
3               1          2
4     12345678901234567890
5               |          |
6     COORDS  =           1
7     EPS     =0.000000001
8     KVAR    =           0
9     FVAR    =           0
10    GVAR    =           0
11    SSTATE  =           1
(12)  DT      =         2.0
(13)  PRNTFR  =          20
(14)  TMAX    =       100.0
15    S1VAR   =           0
16    S3VAR   =           0
17    ELEMS   =           1
18    NELEMS  =          24
19    NNODES  =          21
20    NBSEGS  =          16
```

Part II Element Information

Continuously, next four lines are ignored. For each line of element information contains element number, element type, number of node in element, material number of element, values of k, f, and g for element, counter clockwise node numbers for the element, respectively.

Example

```
ELEMENT INFORMATION:
          1         2         3         4         5
12345678901234567890123456789012345678901234567890123456789012345
   |  |  |  |     D    |     D    |     D    |    |    |    |
   1  1  3  1   25.0        0.0        0.0        1    7    2
   2  1  3  1   25.0        0.0        0.0        2    7    8
   3  1  3  1   25.0        0.0        0.0        2    8    3
   4  1  3  1   25.0        0.0        0.0        3    8    9
   5  1  3  1   25.0        0.0        0.0        3    9    4
   :  :  :  :     :          :          :          :    :    :
   :  :  :  :     :          :          :          :    :    :
```

Part III Nodal Information

Here again, the first four lines are ignored, each line next contains node data, including nodal number, x and y (or r and z) nodal coordinates, and initial value u_0 at the node (option for unsteady state problem).

Example

```
NODAL INFORMATION:
          1         2         3
123456789012345678901234567890123456789012345
    |     D    |     D    |     D    |
    1    0.000      0.003      0.0000
    2    0.001      0.003      0.0000
    3    0.002      0.003      0.0000
    4    0.003      0.003      0.0000
    5    0.004      0.003      0.0000
    :      :          :          :
    :      :          :          :
```

Part IV Node Information

The same as the nodal information, the first four lines are ignored, next line contains boundary segment number, segment type, a number of node in segment, material number of the segment, boundary type (1, 2, and 3 are type S1, S2, or S3), A, B, element number of which segment is part, and node numbers for the segment. Here, "A" means u_1 for S1 type boundary segment, but, for S3 type boundary segment, A and B are values of α and β, respectively.

Example

```
BOUNDARY INFORMATION:
         1         2         3         4         5         6
12345678901234567890123456789012345678901234567890123456789012345678901234567890
    |    |    |    |    |              |              |    |    |    |
    1    1    2    1    2         0.00         0.00    1    1    7
    2    1    2    1    2         0.00         0.00   11    7   13
    3    1    2    1    2         0.00         0.00   21   13   19
    4    1    2    1    2         0.00         0.00   22   19   20
    5    1    2    1    2         0.00         0.00   24   20   21
    :    :    :    :    :            :            :    :    :    :
    :    :    :    :    :            :            :    :    :    :
```

3.3.4 User Instruction

The Program was designed for user with friendly interface of Visual Basic environment. So the user can just create a data file corresponding to a specific problem and follows the direction guide shown with the program interfaces in Appendix B. The result will be exhibited properly. For implementation of the program, the user may create program to build an appropriate data file by selection of his/her own alternative.