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THE MIG2DF COMPUTER CODE USER'S MANUAL

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Hideo KIMURA

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Japan Atomic Energy Research Institute

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The MIG2DF Computer Code User's Manual

Hideo KIMURA

Department of Environmental Safety Research
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura Naka-gun, Ibaraki-ken

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This report describes the MIG2DF computer code and presents the direction to use the code effectively. MIG2DF is a two-dimensional, finite element code simulating saturated-unsaturated groundwater flow and radionuclide transport in porous media for the safety evaluation of radioactive waste disposal. Simulations can be performed in a vertical or horizontal cross-section, or an axisymmetric configuration. Heterogeneities and anisotropy of geologic media are handled by taking advantage of the finite element approach. The equation of groundwater flow is based on the Darcy's law and discretized by the Galerkin finite element method. For the simulations of radionuclide transport, MIG2DF takes account of advection, hydrodynamic dispersion, equilibrium sorption and decay chains. The equations of radionuclide transport are discretized by the Bubnov-Galerkin finite element method.

Keywords: Groundwater Flow, Nuclide Migration, Advection, Dispersion, Finite Element Method, Darcy's Law, Sorption, Saturated-unsaturated, Geologic Media, Radioactive Waste Disposal, Safety Evaluation, Performance Assessment

計算コードMIG2DFのユーザーズマニュアル

日本原子力研究所東海研究所環境安全研究部
木村　英雄

(1992年7月8日受理)

本報告書は、計算コードMIG2DFについて述べたもので、本コードを有効に使うためのユーザーズマニュアルである。MIG2DFは放射性廃棄物地中処分の安全評価を目的として、多孔質媒体中における飽和－不飽和地下水流解析及び核種移行解析を行う2次元有限要素計算コードである。本コードは水平又は鉛直方向2次元断面及び軸対称系における計算が可能である。また有限要素法を採用したため、地質の不均質及び異方性を容易に考慮することが可能である。地下水流の支配方程式はダルシー則に基づいたものであり、Galerkin有限要素法を用いて離散化されている。また核種移行解析では、移流、水文学的拡散、平衡吸着及び崩壊連鎖を考慮することが可能であり、その支配方程式はBubnov-Galerkin（上流型）有限要素法を用いて離散化されている。

東海研究所：〒319-11　茨城県那珂郡東海村白方字白根2－4

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1. Introduction

This report describes the MIG2DF computer code developed by Japan Atomic Energy Research Institute (JAERI) as part of a performance assessment methodology for a radioactive waste repository. The purpose of MIG2DF computer code is to simulate radionuclide transport in groundwater. Transport by groundwater flow is the most likely means of escape for released radionuclide migration in geologic media, therefore the modelling of groundwater flow and radionuclide transport is critically important in the radioactive waste disposal.

MIG2DF is a two-dimensional, finite element code simulating saturated-unsaturated groundwater flow and radionuclide transport in porous media. Simulations can be performed in a vertical or horizontal cross-section, or an axisymmetric configuration. Heterogeneities and anisotropy of geologic media are handled by taking advantage of the finite element approach. Neuman [1)] and Akai et al.[2)] proposed the models which handle saturated-unsaturated seepage problem using finite element method. The same method is used for groundwater flow analysis in MIG2DF code. Many types of boundary conditions can be accommodated: 1) water table conditions, 2) atomospheric conditions associated with seepage boundaries and infiltration, 3) pumping and injection wells. For radionuclide transport simulation, MIG2DF takes account of advection, hydrodynamic dispersion, equilibrium sorption and decay chain. Up-stream weighting method is used to eliminate osillations of numerical solutions when a convective transport dominates the dispersive transport. The scheme can accommodate straight and branch decay chains. Arbitrary release-patterns of radionuclides from sources can be handled.

The equation of groundwater flow is based on the Darcy's law and discretized by using the Galerkin finite element method. The equations of radionuclide transport are discretized by using the Bubnov-Galerkin finite element method.

MIG2DF is written in ANSI Standard FORTRAN 77 and can be compiled on any standard computer system. Installation of code has been made on FACOM M-780 mainframe system, and MIPS and IBM workstations with standard FORTRAN compilers.

2. Governing equations

In the modelling of groundwater flow and radionuclide transport, the basic equations are given by the following three equations.

(1) The continuity equation which expresses mass conservation of fluid.

(2) The Darcy's law for porous media which expresses momentum conservation.

(3) The radionuclide transport equation which expresses mass conservation of solute.

1. Introduction

This report describes the MIG2DF computer code developed by Japan Atomic Energy Research Institute (JAERI) as part of a performance assessment methodology for a radioactive waste repository. The purpose of MIG2DF computer code is to simulate radionuclide transport in groundwater. Transport by groundwater flow is the most likely means of escape for released radionuclide migration in geologic media, therefore the modelling of groundwater flow and radionuclide transport is critically important in the radioactive waste disposal.

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(3) The radionuclide transport equation which expresses mass conservation of solute.

Mass conservation of fluid

The continuity equation in a porous medium can be written.

$$\frac{\partial}{\partial t}(\phi\rho_f) + div\,(\rho_f\vec{u}) = Q_f \tag{1}$$

where
ϕ is the volumetric water content (-)
ρ_f the fluid density (kg/m^3)
$\vec{u}$ the Darcy flow velocity (m/sec)
t time (sec)
and Q_f the source or sink strength of fluid (kg/m^3 sec)

The first term of equation (1) can be rewritten as follows using pressure head h_p (m)

$$\frac{\partial}{\partial t}(\phi\rho_f) = \rho_f[C + S\rho_0 g(\alpha+\varepsilon\beta)]\frac{\partial h_p}{\partial t} \equiv \rho_f C'\frac{\partial h_p}{\partial t} \tag{2}$$

$$C' = C = \varepsilon\frac{\partial S}{\partial h_p} \qquad \text{(unsaturated case)} \tag{3}$$

$$C' = S_W = S\rho_0 g(\alpha+\varepsilon\beta) \qquad \text{(saturated case)} \tag{4}$$

where
C is the specific moisture capacity (1/m)
S the saturation rate of water (-) ($\phi = \varepsilon S$, $0 \le S \le 1$)
ρ_0 the fluid density at a reference temperature
g gravitational acceleration (m/sec^2)
α the compressibility of rock (m^2/N)
β the compressibility of water (m^2/N)
ε the porosity of rock (-)
and S_W the specific storage (1/m)

The specific moisture capacity C is zero for saturated case because the saturation rate S is constant for a increment of pressure head h_p. The effect of water and rock/soil compressibility on the storage of water under unsaturated conditions are usually quite small compared to the effect of changes in S, and therefore the specific storage S_W can be neglected for unsaturated case.

Momentum conservation

The Darcy's equation is commonly adopted for the motion of groundwater flow in a porous medium

$$\vec{u} = -\mathbf{K}_f[\nabla(h_p + h_e) - \vec{e}_z\frac{\rho_f - \rho_0}{\rho_0}] \tag{5}$$

where $\mathbf{K}_f$ is the hydraulic conductivity tensor (m/sec)
h_e the elevation head pressure (m)
and $\vec{e}_z$ unit vector in a gravitational direction (-)

Note that $\mathbf{K}_f$ is generally the function of temperature and is also the function of pressure head in unsaturated cases. We must consider similar equation for air in unsaturated porous media. However, if we assume that the air is stationary or ignore its movement, eq. (5) is valid for unsaturated porous media.[3)]

Mass conservation of solute

Transport of a chain of decaying solute species is described by the following equation considering advection, dispersion[4), 5)] and adsorption on the surface of a solid:

$$\begin{aligned}\nabla(\mathbf{D}\nabla C_k - \vec{u}C_k) &= \frac{\partial}{\partial t}[\phi C_k + \rho_S(1-\varepsilon)C_{S,k}] + \lambda_k[\phi C_k + \rho_S(1-\varepsilon)C_{S,k}] \\ &\quad - \sum_{m=1}^{k-1} \xi_{km}\lambda_m[\phi C_m + \rho_S(1-\varepsilon)C_{S,m}] - Q_k\end{aligned} \tag{6}$$

$$D_{ij} = D_T|\vec{u}|\delta_{ij} + (D_L - D_T)\frac{u_i u_j}{|\vec{u}|} + \phi D_d \tau \delta_{ij} \tag{7}$$

where	$\mathbf{D}$	is the hydrodynamic dispersion tensor (m^2/sec)
	C_k	the concentration of radionuclide k in groundwater (kg/m^3)
	ρ_S	the density of solid (kg/m^3)
	$C_{S,k}$	the adsorbed concentration of radionuclide k (kg/m^3)
	λ_k	decay constant of radionuclide k (1/sec)
	ξ_{km}	the mass fraction of radionuclide m (parent) transforming to k (daughter) (-)
	Q_k	source term of radionuclide k (kg/m^3sec)
	D_T	transverse dispersion length (m)
	D_L	longitudinal dispersion length (m)
	D_d	the molecular diffusion coefficient in a free-water (m^2/sec)
	and τ	tortuosity.

Assuming that the relation between adsorbed and solution concentration is described by a linear equilibrium isotherm, eq. (6) can be expressed as

$$\nabla(\mathbf{D}\nabla C_k - \vec{u}C_k) = \frac{\partial}{\partial t}[\phi(1 + \frac{\rho_S(1-\varepsilon)Kd_k}{\phi})C_k] + \lambda_k[\phi(1 + \frac{\rho_S(1-\varepsilon)Kd_k}{\phi})C_k] - \sum_{m=1}^{k-1}\xi_{km}\lambda_m[\phi(1 + \frac{\rho_S(1-\varepsilon)Kd_m}{\phi})C_m] - Q_k \tag{8}$$

where Kd_k is the equilibrium constant.

Equation (8) reduces to

$$\nabla(\mathbf{D}\nabla C_k - \vec{u}C_k) = \frac{\partial}{\partial t}[\phi R_k C_k] + \lambda_k \phi R_k C_k - \sum_{m=1}^{k-1}\xi_{km}\lambda_m \phi R_m C_m - Q_k \tag{9}$$

where R_k is the retardation factor defined as

$$R_k = 1 + \frac{\rho_S(1-\varepsilon)Kd_k}{\phi} . \tag{10}$$

3. Initial and boundary conditions

The initial condition of saturated-unsaturated groundwater flow problem is

$$h_p(x,0) = h_p^0(x) \tag{11}$$

where $h_p^0(x)$ is the initial head value.

The following three kinds of boundary conditions are assigned in the saturated-unsaturated groundwater flow problem. Treatments of seepage boundaries in this model are same as those of 3D-SEEP[6)] and 2D-SEEP[7)] codes.

(1) A prescribed hydraulic pressure head on a surface

$$h_p = \bar{h}_p \tag{12}$$

(2) A prescribed water flux normal to a surface

$$u_n = \bar{u}_n \tag{13}$$

(3) Atmospheric boundary where the relationship between velocity and moisture is prescribed

$$u_n + \bar{q}_r = 0 \qquad \text{(unsaurated)} \tag{14}$$

$$h_p = 0 \qquad \text{(saturated)} \tag{15}$$

where $\bar{q}_r$ is rainfall recharge (m/sec).

For the radionuclide transport problem, the following initial condition is assigned.

$$C_k(x,z,0) = \tilde{C}_k(x,z) \tag{16}$$

where $\tilde{C}_k$ is the initial concentration of radionuclide k.

The boundary conditions of the radionuclide transport problem are as follows:

(4) A prescribed concentration on a surface Γ_1

$$C_k = \overline{C}_k \qquad \text{on } \Gamma_1 \tag{17}$$

(5) Prescribed solute mass fluxes on surfaces Γ_2 and Γ_3

$$q_{nk} = -\mathbf{n}\cdot\ \overline{D}\,\mathrm{grad}C_k \qquad \text{on } \Gamma_2 \tag{18}$$

$$q_{nk} = \mathbf{n}\cdot\ (\mathbf{u}C_k - \overline{D}\,\mathrm{grad}C_k) \qquad \text{on } \Gamma_3 \tag{19}$$

4. Discretization by finite element method

Groundwater flow

The Galerkin finite element method is employed for the grounwater flow equations. For an arbitrary value of δh_p , the following equation must be satisfied from eqs. (1) and (2).

$$\int_V (\nabla\cdot\ (\rho_f\vec{u}) - Q_f + \rho_f C'\frac{\partial h_p}{\partial t})\delta h_p dV = 0 \tag{20}$$

By using the divergence theorem this can be rearranged into the form of a volume integral plus a boundary term

$$\int_V [\,-\,\rho_f\vec{u}\cdot\nabla\ (\delta h_p) + (\rho_f C'\frac{\partial h_p}{\partial t} - Q_f)\delta h_p]dV + \int_S \rho_f u_n \delta h_p dS = 0 \tag{21}$$

The pressure head is assumed to be the linear combination of known shape functions $N_i(\mathbf{r})$.

$$h_p = \sum_i h_p^i(t)\cdot\ N_i(\mathbf{r}) \tag{22}$$

$$\delta h_p = \sum_i \delta h_p^i(t)\cdot\ N_i(\mathbf{r}) \tag{23}$$

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$$\delta h_p = \sum_i \delta h_p^i(t)\cdot N_i(\mathbf{r}) \tag{23}$$

Substituting equations (5), (22) and (23) into eq. (21)

$$\delta h_p^i \left\{ \int_V \left[\nabla N_i \cdot \left(\rho_f \mathbf{K}_f \cdot \sum_j \nabla N_j h_p^j\right) + \nabla N_i \cdot \left(\rho_f \mathbf{K}_f \frac{\rho_0 - \rho_f}{\rho_0} \vec{e}_z\right) + N_i\left(\rho_f C' \frac{\partial h_p}{\partial t} - Q_f\right)\right] dV \right\} + \delta h_p^i \int_S N_i \rho_f u_n dS = 0 \tag{24}$$

For arbitrarily chosen δh_p^i and h_p^j , {h} must satisfy the following equation.

$$[K]\{h\} + \{B\} - \{Q\} + \{q\} + [E]\left\{\frac{\partial h}{\partial t}\right\} = 0 \tag{25}$$

where $$K_{ij} \equiv \int_V \nabla N_i \cdot (\rho_f \mathbf{K}_f \cdot \nabla N_j) dV \tag{26}$$

$$B_i \equiv \int_V \nabla N_i \cdot \left(\rho_f \mathbf{K}_f \frac{\rho_0 - \rho_f}{\rho_0} \vec{e}_z\right) dV \tag{27}$$

$$Q_i \equiv \int_V N_i Q_f dV \tag{28}$$

$$q_i \equiv \int_S N_i \rho_f u_n dS \tag{29}$$

$$E_{ij} \equiv \int_V N_i \rho_f C' N_j dV \tag{30}$$

Radionuclide transport

The Bubnov-Galerkin finite element method is employed for radionuclide transport equations. For an arbitrary value of δC_k, the following equation must be satisfied from eq. (9).

$$\int_V \delta C_k[\phi R_k\frac{\partial C_k}{\partial t} - \nabla(\mathbf{D}\nabla C_k - \vec{u}C_k) + \phi R_k\lambda_k C_k$$
$$- \sum_{m=1}^{k-1} \xi_{km}\lambda_m\phi R_m C_m - Q_k]dV = 0 \tag{31}$$

which assuming that the time derivative of (ϕR_k) is neglected. By using the divergence theorem this can be rearranged into the form of a volume integral plus a boundary term

$$\int_V \delta C_k\phi R_k\frac{\partial C_k}{\partial t} - \int_S [\phi\mathbf{D}\nabla C_k]\cdot\vec{n}\delta C_k dS$$
$$- \int_V [D\nabla C_k - \vec{u}C_k]\nabla\delta C_k dV + \int_V \delta C_k\phi R_k\lambda_k C_k dV$$
$$- \int_V \delta C_k\sum_{m=1}^{k-1} \xi_{km}\lambda_m\phi R_m C_m dV - \int_V \delta C_k Q_k dV = 0. \tag{32}$$

The concentration of radionuclide is assumed to be the linear combination of known shape functions $N_i(\mathbf{r})$ or weighting functions $\omega_i(\mathbf{r})$. The up-stream weighting functions $\omega_i(\mathbf{r})$ are used for convective terms of eq. (32).

$$C_k = \sum_i C_k^i(t)\cdot N_i(\mathbf{r}) \tag{33}$$

$$\delta C_k = \sum_i \delta C_k^i(t)\cdot N_i(\mathbf{r}) \tag{34}$$

$$\text{or } = \sum_i \delta C_k^i(t)\cdot \omega_i(\mathbf{r}) \qquad \text{(for convective term)} \tag{35}$$

Substituting equations (33), (34) and (35) into eq. (32), and finally the following equation are obtained.

$$[T]\{\frac{\partial C_k}{\partial t}\} + \{[A] + [U] + [G] + [S_2]\}\{C_k\} + \{q_3\} + \{q_2\} + \{Q\} + \{d\} = 0 \tag{36}$$

where $$T_{ij} \equiv \int_V \phi R_k N_i N_j dV \tag{37}$$

$$A_{ij} \equiv \int_V \nabla \omega_i \mathbf{D} \nabla N_j dV \tag{38}$$

$$U_{ij} \equiv -\int_V \nabla \omega_i \vec{u} N_j dV \tag{39}$$

$$G_{ij} \equiv \int_V \lambda_k \phi R_k N_i N_j dV \tag{40}$$

$$S_{2ij} \equiv \int_{S_{2'}+S_2} \vec{u} \cdot \vec{n}\, \omega_i N_j dS + \int_{S_2} \omega_i \vec{n} \mathbf{D} \begin{Bmatrix} -1 \\ n_x/n_y \end{Bmatrix} \frac{\partial N_j}{\partial x} dS \tag{41}$$

$$q_{3i} \equiv \int_{S_1+S_3} \omega_i q_n dS \tag{42}$$

$$q_{2i} \equiv \int_{S_{2'}} \omega_i q_n dS + \int_{S_2} \omega_i \vec{n} \mathbf{D} \begin{Bmatrix} 0 \\ q_n/n_y \end{Bmatrix} dS \tag{43}$$

$$Q_i \equiv -\int_V N_i Q_k dV \tag{44}$$

$$d_i \equiv -\sum_{m=1}^{k-1} \int_V \xi_{km} \lambda_m \phi R_m N_i N_j dV \cdot C_{mj} \tag{45}$$

5. Finite element

Two types of finite element are used in this model. One is a linear triangular element, and a square element is treated as a composite element which is composed of two triangular elements. The another is an isoparametric square element which is made up of variable nodes between four and eight.

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Linear triangular element

Triangular elements are made up of three nodes, and are only used for groundwater flow analysis. The shape functions of this element are given as follows. (see Fig.1)

$$N_i(x,y) = \frac{A_i}{A} \qquad (46)$$

where

$$A_i = \frac{1}{2}\begin{vmatrix} 1 & x & y \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{vmatrix} \qquad (\, i = 1, 2, 3 \,) \quad (\, (i, j, k) \text{ is even permutation of } (1, 2, 3) \,) \qquad (47)$$

$$A = \frac{1}{2}\begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} \qquad (\text{ area of triangular element }) \qquad (48)$$

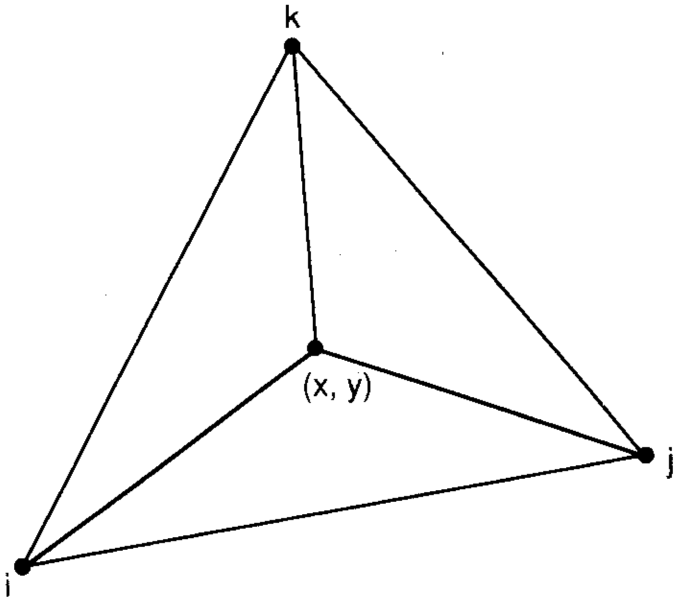


Fig. 1 Linear triangular element

Composite element (square element)

Square elements are divided into two sets of triangular elements as shown in Fig. 2. The physical values of this element are given by superposing and averaging those of each triangular element. This element also can not be used for the radionuclide transport problem.

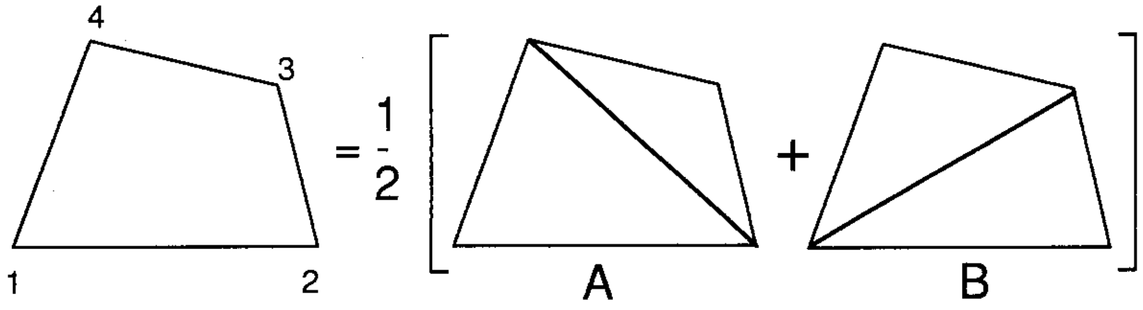


Fig. 2 Treatment of composite element

Isoparametric element

Isoparametric elements of this model are made up of variable nodes between four and eight as shown in Fig. 3. Triangular isoparametric elements are treated by degenerating node of the third vertex and that of fourth as shown in Fig. 4.

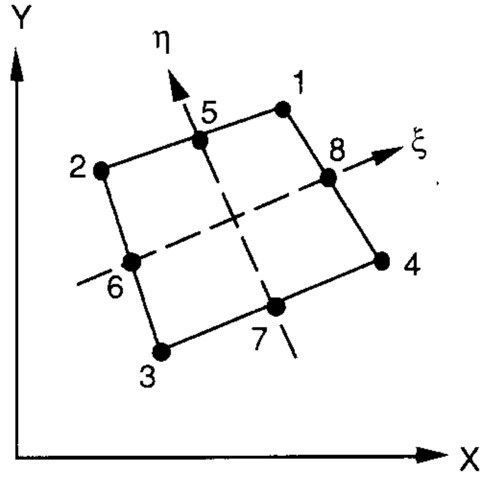


Fig. 3 Isoparametric element

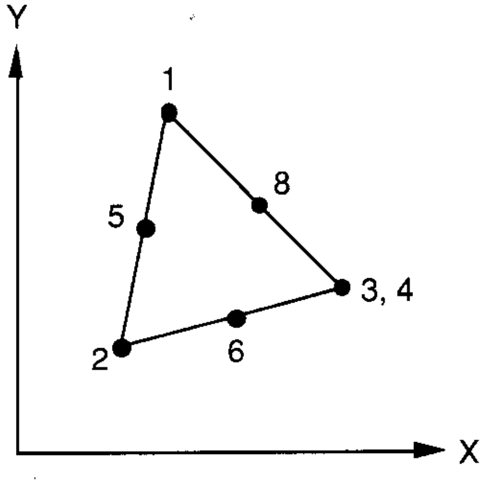


Fig.4 Treatment of triangular element

The shape functions N_i are

$$N_1 = \frac{1}{4}(1+\xi)(1+\eta) - N_5/2 - N_8/2 \tag{49-1}$$

$$N_2 = \frac{1}{4}(1-\xi)(1+\eta) - N_5/2 - N_6/2 \tag{49-2}$$

$$N_3 = \frac{1}{4}(1-\xi)(1-\eta) - N_6/2 - N_7/2 \tag{49-3}$$

$$N_4 = \frac{1}{4}(1+\xi)(1-\eta) - N_7/2 - N_8/2 \tag{49-4}$$

$$N_5 = \frac{1}{2}(1-\xi^2)(1+\eta) \tag{49-5}$$

$$N_6 = \frac{1}{2}(1-\xi)(1-\eta^2) \tag{49-6}$$

$$N_7 = \frac{1}{2}(1-\xi^2)(1-\eta) \tag{49-7}$$

$$N_8 = \frac{1}{2}(1+\xi)(1-\eta^2) \tag{49-8}$$

where ξ and η are intrinsic coordinates.

Up-stream test functions

The up-stream test functions are given for the square four noded isoparametric elements as follows.

$$\omega_1 = \frac{1}{16}[\, f(\xi) + 3\alpha_1(\xi^2 - 1)\,][\, f(\eta) + 3\beta_2(\eta^2 - 1)\,] \tag{50-1}$$

$$\omega_2 = \frac{1}{16}[\, g(\xi) + 3\alpha_1(1 - \xi^2)\,][\, f(\eta) + 3\beta_1(\eta^2 - 1)\,] \tag{50-2}$$

$$\omega_3 = \frac{1}{16}[\, g(\xi) + 3\alpha_2(1 - \xi^2)\,][\, g(\eta) + 3\beta_1(1 - \eta^2)\,] \tag{50-3}$$

$$\omega_4 = \frac{1}{16}[\, f(\xi) + 3\alpha_2(\xi^2 - 1)\,][\, g(\eta) + 3\beta_2(1 - \eta^2)\,] \tag{50-4}$$

where $f(x) \equiv 2(1 - x)$, $g(x) \equiv 2(1 + x)$

α_n, β_n : up-stream weighting parameters (=0 normal Galerkin weighting)

Parameters α_n and β_n are computed taking appropriate values of local Reynolds numbers γ defined by equation (51) along appropriate element sides and directions.[8]

$$\gamma_x = \frac{u_x \Delta x}{D_x}, \quad \gamma_y = \frac{u_y \Delta y}{D_y} \tag{51}$$

where Δx the mesh size in the x direction

Δy	the mesh size in the y direction
u_x	the velocity of x-component along an element side
u_y	the velocity of y-component along an element side
D_x	the dispesion coefficient in the x direction
and D_y	the dispesion coefficient in the y direction.

The signs of α_n and β_n depend on the direction of velocities as shown in Fig. 5.

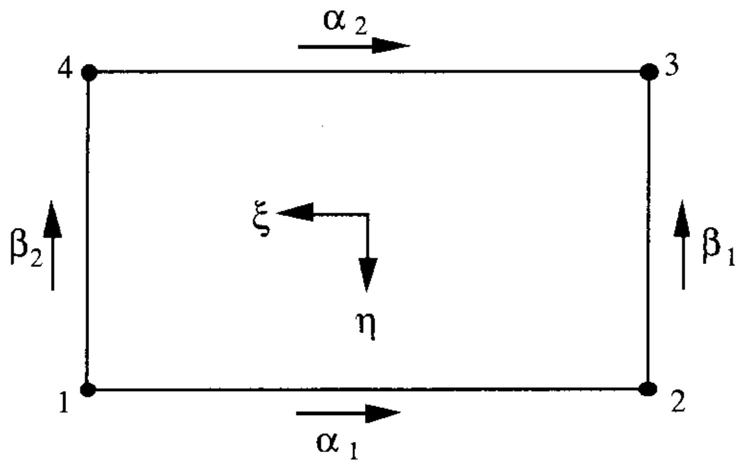


Fig. 5 Up-stream parameters of 4 node element

As in a general case, the velocities will be variable (as well as the conductivities and mesh); the component of the average velocity vector along the element side is calculated by the following equations.

$$v_{ij} = \frac{1}{2}(\vec{u}_i + \vec{u}_j)^T \cdot \vec{l}_{ij} \tag{52}$$

where	$\vec{u}_i$	the velocity of node i
	$\vec{u}_j$	the velocity of node j
	and $\vec{l}_{ij}$	a unit vector in the direction between node i and node j.

The signs of α_n and β_n are determined by the sign of v_{ij} in equation (52).

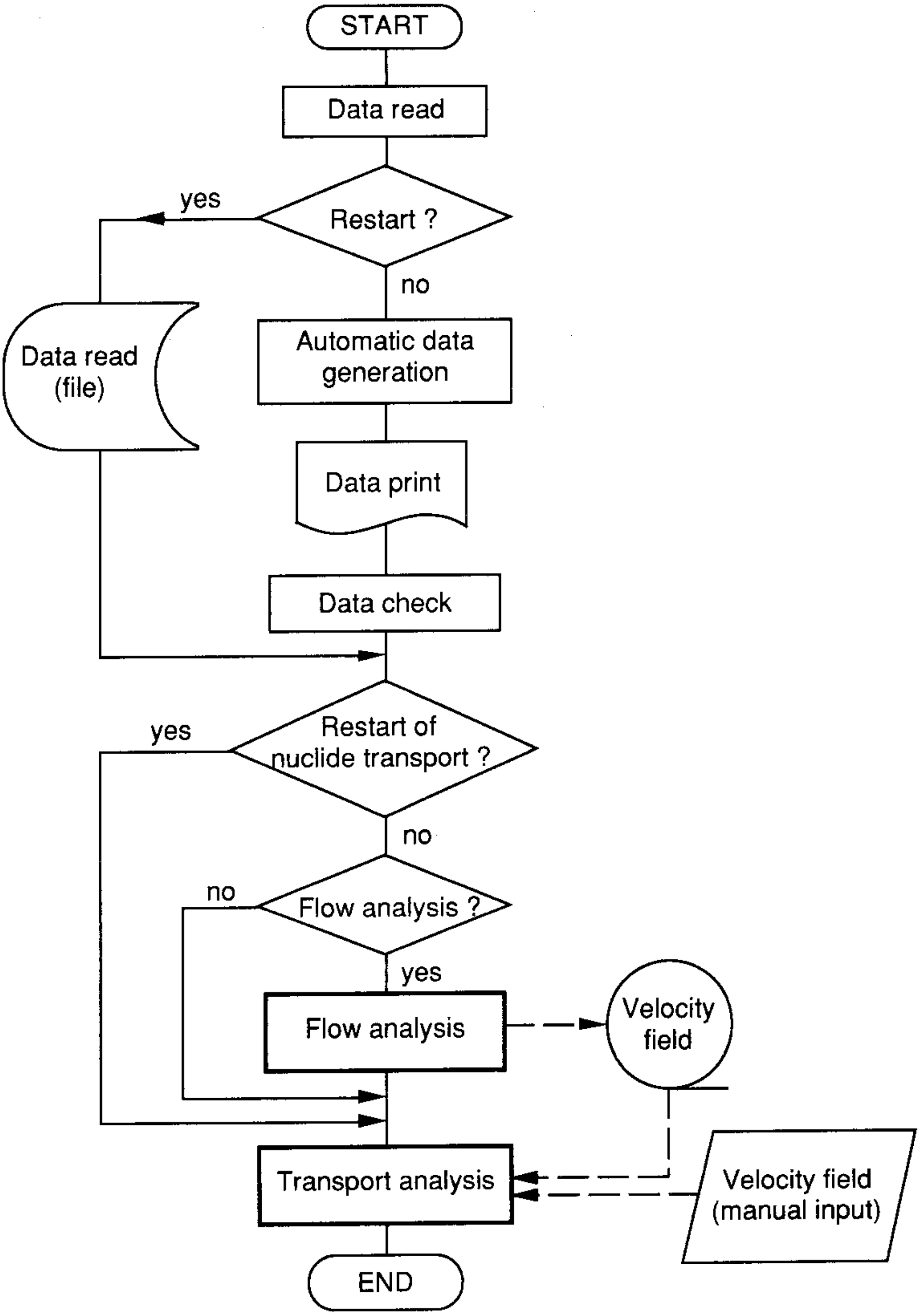


Fig. 6 Flow chart of MIG2DF code

6. Numerical method

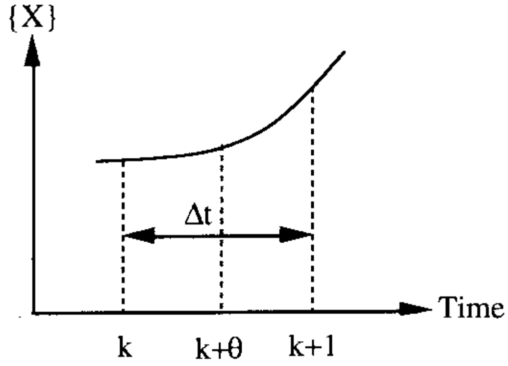
Flow chart of this model is shown in Fig. 6. Equations (25) and (36) to be solved can be written in the following matrix form.

$$[A]\left\{\frac{\partial X}{\partial t}\right\}+[B]\{X\}=\{f\} \tag{53}$$

For a transient state analysis, the generalized Crank-Nicholson method is adopted for the discretization of time.

$$\left\{\frac{\partial X}{\partial t}\right\}^{k+\theta}=\frac{1}{\Delta t}(\{X\}^{k+1}-\{X\}^{k}) \tag{54}$$

$$\{X\}^{k+\theta}=\frac{1-\theta}{2}\{X\}^{k}+\frac{1+\theta}{2}\{X\}^{k+1} \tag{55}$$



where k is time step

and θ Crank-Nicholson parameter. ($-1 \leq \theta \leq 1$)

Substituting equations (54) and (55) into eq. (53), we can get the following equations.

$$[B']\{X\}^{k+1}=\{f'\} \tag{56}$$

where
$$[B']\equiv\frac{[A]^{k+\theta}}{\Delta t}+\frac{1+\theta}{2}[B]^{k+\theta} \tag{57}$$

$$\{f'\}\equiv\{f\}^{k+\theta}+(\frac{[A]^{k+\theta}}{\Delta t}-\frac{1-\theta}{2}[B]^{k+\theta})\{X\}^{k} \tag{58}$$

The set of equations in eq. (56) is solved by the direct method with band memorization schemes. As the matrix [B'] and the load vector {f'} of eq. (56) are the function of pressure head in the case of groundwater flow analysis, the equation becomes non-linear. Equation (56) is solved by using the following iterative method. We assume

$$\{X\}^{k+1} = (1-v)\{X\}_r^{k+1} + v\{X\}_{r+1}^{k+1} \tag{59}$$

$$[B'] = (1-v)[B']_{r-1} + v[B']_r \tag{60}$$

$$\{f'\} = (1-v)\{f'\}_{r-1} + v\{f'\}_r \tag{61}$$

where v is coefficient of acceleration, and suffix r and r+1 denote previous and present iteration levels at the current time step. Substituting equation (59) into eq. (56),

$$v[B']\{X\}_{r+1}^{k+1} = \{f'\} - (1-v)[B']\{X\}_r^{k+1}. \tag{62}$$

Equations (59), (60), (61) and (62) are iteratively solved until the successive change in the value of {X} is within a prescribed tolerance.

The structure of computer code MIG2DF is divided into parts of groundwater flow and radionuclide transport. Four kinds of simulation are possible, the first three are simulations of groundwater flow, and the last one is simulation of radionuclide transport:

1) steady state flow analysis,
2) transient state flow analysis,
3) steady state flow analysis and continuous transient state flow analysis,
4) transient state analysis of radionuclide transport.

In the simulation of radionuclide transport, a velocity of groundwater flow is assumed to be constant in a finite element. Various forms of velocity data are available in the simulations:

1) velocities calculated from this code,
2) manually given velocities (user-file),
3) velocities calculated from analytical solutions (user-subroutine).

Restart runs of the simulations are possible in all cases above mentioned in order to save the computational sizes.

Acknowledgment

The author would like to express his gratitude to Mr. H. Matsuzuru, Mr. S. Shima, Mr. M. Munakata and Mr. N. Kato for helpful discussions and advice.

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8) Zienkiewicz, O. C. and Heinrich, J. C., 1978, The finite element method and convection problems in fluid mechanics, 'Finite Elements in Fluids Vol. 3', John Wiley & Sons.

Acknowledgment

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References

1) Neuman, S. P., 1973, Saturated unsaturated seepage by finite elements, Proc. ASCE, vol. 99, No. HY12, p.2233~2250.

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3) Bear, J. and Verruijt, A., 1987, Modelling Groundwater Flow and Pollution, Reidel.

4) Scheidegger, A. E., 1961, Generalized theory of dispersion in porous media, J. Geophys. Res. vol. 66, p.3273~3278.

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7) Kimura, H., 1988, The 2D-SEEP computer code user's manual, JAERI-M 88-132.

8) Zienkiewicz, O. C. and Heinrich, J. C., 1978, The finite element method and convection problems in fluid mechanics, 'Finite Elements in Fluids Vol. 3', John Wiley & Sons.

Appendix 1 Input data for MIG2DF

MIG2DF code includes plotting subroutines which plot the numerical results of groundwater flow and radionuclide transport. Input data are composed of two types of data: 1) input data for the simulation of groundwater flow and radionuclide transport, 2) input data for plotting. (see Fig. A-1)

I. Input data for groundwater flow and radionuclide transport

1. Job Identification Card

This card is used for the identification of computational jobs which involve flow and transport simulations ('SEEPNUCL') and plottings of numerical results ('PLOTSEEP' and 'HISTORY').

Column	entry	contents	format
1 ~ 4	'STEP'		A4
11 ~ 18		enter 'SEEPNUCL'	2A4

2. Title Card

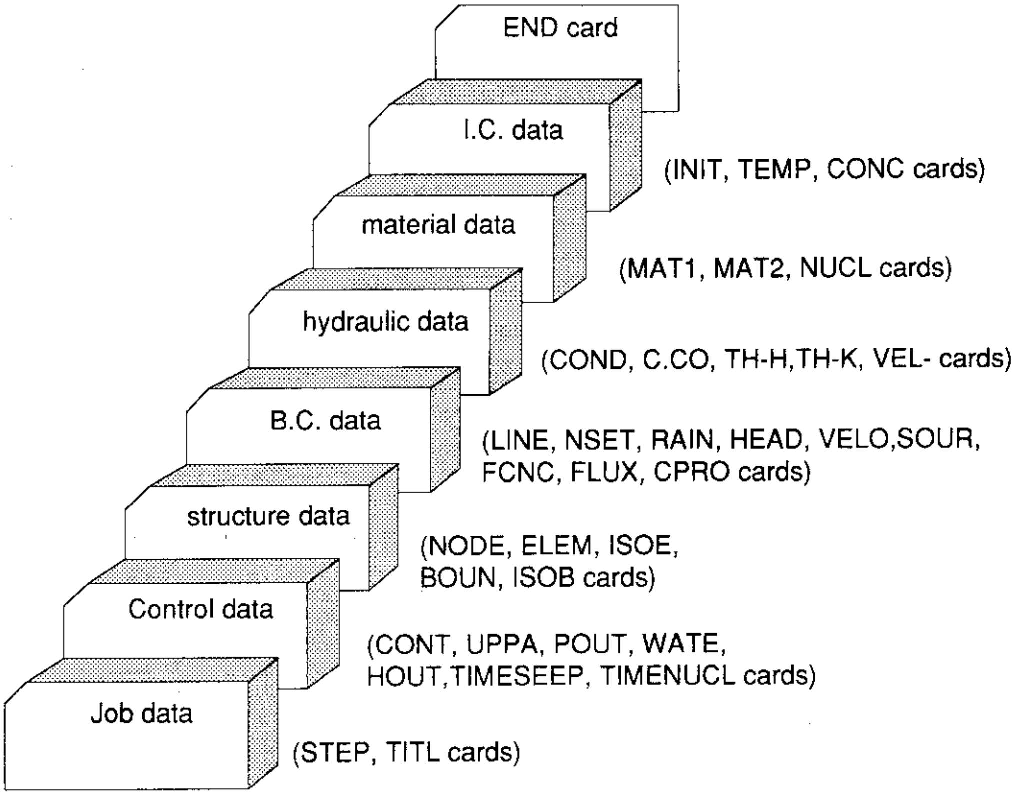
Title name of the computational job is inputted by this card, and the title will be printed out in all pages of the output-list.

Column	entry	contents	format
1 ~ 4	'TITL'		A4
11 ~ 74		enter 'Title name'	16A4

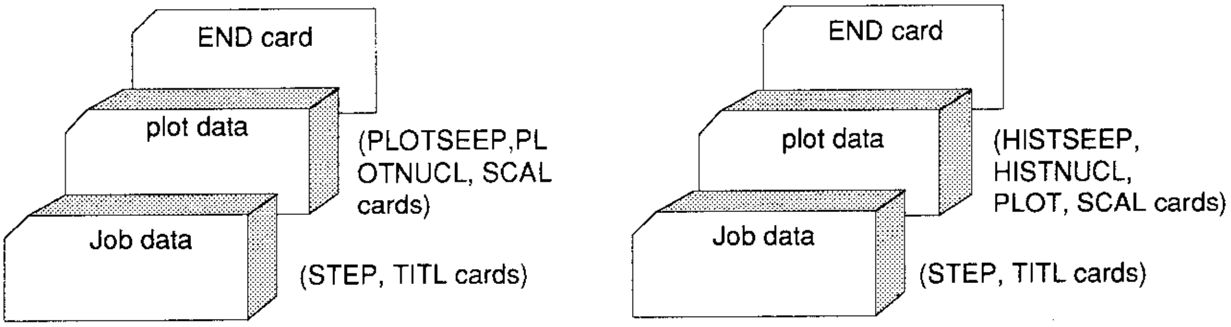
3. Comment Card

This card is used for comment of input data, and it may be inserted anywhere.

Column	entry	contents	format
1 ~ 4	'****'	meaning of comment card	A4
5 ~ 80		enter 'Comment'	



simulation of groundwater flow and radionuclide transport



plotting of mesh, contour and vector

plotting of histoty data

Fig. A-1 Input data for MIG2DF

4. Control Card

These data specify conditions of the computational job.

Column	entry	contents	format
1 ~ 4	'CONT'	meaning of control card	A4
11 ~ 12	I1	=1:normal run, =2:restart run (using structure file), =3:restart run (using structure and results files)	I2
13 ~ 14	I2	interval of printout for transient analysis	I2
15 ~ 16	I3	total maximum number of iterations	I2
17 ~ 18	I4	=1:steady state flow analysis, =2:transient state flow analysis, =3:steady + transient flow analysis, =60-66:nuclide transport analysis *	I2
19 ~ 20	I5	=1:vertical domain, =2:horizontal domain, =3:axial symmetry domain	I2
21 ~ 22	I6	=1:band minimize, =0:without band minimize	I2
23 ~ 24	I7	maximum number of iterations in one B.C.	I2
25 ~ 26	I8	maximum number of alternating B.C.	I2
27 ~ 28	I9	flag of automatic element data generations (=1:composite, =2:composite+isoparametric, =3:isoparametric)	I2
29 ~ 30	I10	=1:consider buoyancy effect (=0:not consider)	I2
31 ~ 32	I11	=2:data check run, =0:normal run	I2
33 ~ 34	I12	degree of Gaussian integration (1 ~ 3)	I2
35 ~ 36	I13	control parameter of convergence-check =0:use averaged value for all nodal points, =1:use maximum value of nodal points	I2
37 ~ 38	I14	=0:print out of card-image input data, =1:without print	I2
39 ~ 40	I15	=0:print out of nodal data, =1:without print out	I2
41 ~ 42	I16	=0:print out of element data, =1:without print out	I2
43 ~ 44	I17	=0:groundwater flow analysis, =1:heat conduction	I2
45 ~ 46	I18	initial temperatures for groundwater flow analysis =0:not given, =1:given by steady state analysis (file) =2:given by transient state analysis (file)	I2
47 ~ 50	I19	previous time step (case of restart run I1=3)	I4
51 ~ 55	R1	value for judgement of convergence-check	F5.0
56 ~ 60	R2	coefficient of acceleration (non-linear case)	F5.0
61 ~ 70	R3	compressibility of water	F10.0
71 ~ 72	I20	=0:consider non-linearity in a time-step, =1:not consider	I2
73 ~ 77	I21	time-step of temperature analysis for file-input (I18=2)	I5
78 ~ 80	I22	=1:material data are given by file	I3

* In the nuclide transport analysis, I4 indicates the following job-steps.

flag No. (I4)	input of structural data		input of groundwater flow velocity data				nuclide concentration	
	card	file	calculated by input data	result-file of flow analysis	user-file	user-subroutine	initial run	restart run
60	○	×	○	×	×	×	○	×
61	○	×	×	○	×	×	○	×
62	○	×	×	×	○	×	○	×
63	○	×	×	×	×	○	○	×
64	×	○	×	○	×	×	×	○
65	×	○	×	×	○	×	×	○
66	×	○	×	×	×	○	×	○

5. Up-stream weighting Identification Data

Column	entry	contents	format
1 ~ 4	'UPPA'		A4
11 ~ 20	U1	up-stream weighting factor α_1	F10.0
21 ~ 30	U2	up-stream weighting factor β_1	F10.0
31 ~ 40	U3	up-stream weighting factor α_2	F10.0
41 ~ 50	U4	up-stream weighting factor β_2	F10.0
51 ~ 55	I1	=0:no up-stream weighting, =1:up-stream weighting	I5
56 ~ 65	R1	Crank-Nicholson parameter ($-1<R1<1$)	F10.0
71 ~ 75	I2	=0:no lumping, =1:lumping	I5

6. Output Identification Data

Column	entry	contents	format
1 ~ 4	'POUT'		A4
11 ~ 15	N	number of output items	I5
16 ~ 65	K1 ~K10	output items (maximum =10) =1:pressure head, =2:total head, =3:water content, =4:saturation rate, =5:temperature, =6:averaged Darcy velocity in an element, =7:averaged real velocity in an element, =8:Darcy velocity at a nodal point, =9:water flux at boundary, =100+n:concentration of n-th radionuclide	10I5

7. Fluid Property Data

Column	entry	contents	format
1 ~ 4	'WATE'		A4
11 ~ 20	R1	gravitational acceleration g	F10.0
21 ~ 30	R2	density of water at reference temperature	F10.0
31 ~ 40	R3	specific heat of water	F10.0
41 ~ 50	R4	compressibility of water	F10.0
51 ~ 55	I1	=0:viscosity of water is constant =n:function No. of viscosity defined by user-routine	I5

8. Output Identification Data for History of Concentration

Column	entry	contents	format
1 ~ 4	'HOUT'		A4
9 ~ 10	II	nuclide No.	I2
11 ~ 15	N	number of node for print out (No. of following items)	I5
16 ~ 65	K1 ~K10	node number for print out if N>10, another card is necessary (Max=100)	10I5

9. Time Step Data for Groundwater Flow

1-st Card

Column	entry	contents	format
1 ~ 8	'TIMESEEP'	for transient analysis of groundwater flow	2A4
11 ~ 70	T(1) ~T(n)	1-st output time n-th output time	12F5.0

2-nd Card

Column	entry	contents	format
1 ~ 8	'TIMESEEP'		2A4
11 ~ 65	T(1) ~T(n)	number of time step from T(1) to T(2) number of time step from T(n-1) to T(n)	11F5.0

10. Time Step Data for Nuclide Transport

1-st Card

Column	entry	contents	format
1 ~ 8	'TIMENUCL'	for transient analysis of nuclide transport	2A4
11 ~ 70	T(1) ~T(n)	1-st output time n-th output time	12F5.0

2-nd Card

Column	entry	contents	format
1 ~ 8	'TIMENUCL'		2A4
11 ~ 65	T(1) ~T(n)	number of time step from T(1) to T(2) number of time step from T(n-1) to T(n)	11F5.0

11. Node Data

Header Card of Node Data

Column	entry	contents	format
1 ~ 4	'NODE'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'NODE'		A4
10 ~ 15	N	node number	I5
21 ~ 30	XX	X-coordinate of node	F10.0
31 ~ 40	YY	Y-coordinate of node	F10.0
41 ~ 45	L1	condition No. of nodal water flux (blank:no flux), related to SOUR card	I5
46 ~ 50	L2	condition No. of pressure head (blank:no restriction), related to HEAD card	I5
51 ~ 55	K1	condition No. of nuclide flux (blank:no flux), related to CPRO card	I5
56 ~ 60	K2	condition No. of nuclide concentration (blank:no restriction), related to FCNC card	I5
66 ~ 70	M	increment of node number for automatic generation (blank or 0:without automatic generation)	I5

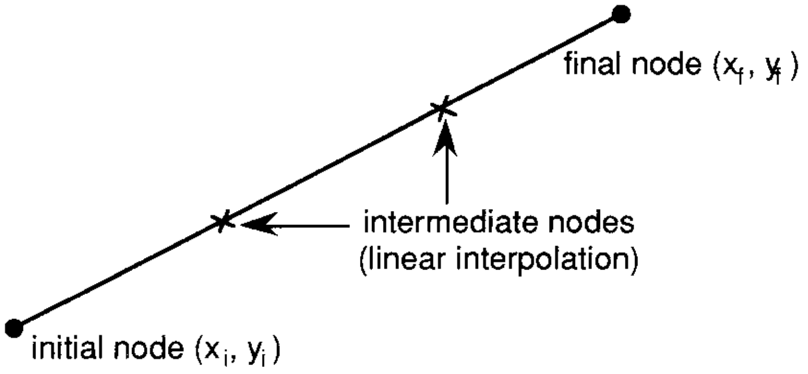


Fig. A-2 Automatic Generation of Node Data

2-nd Card of Node Data

Column	entry	contents	format
1 ~ 4	'NODE'		A4
10 ~ 15	N	node number	I5
21 ~ 30	XX	X-coordinate of node	F10.0
31 ~ 40	YY	Y-coordinate of node	F10.0
41 ~ 80	blank		

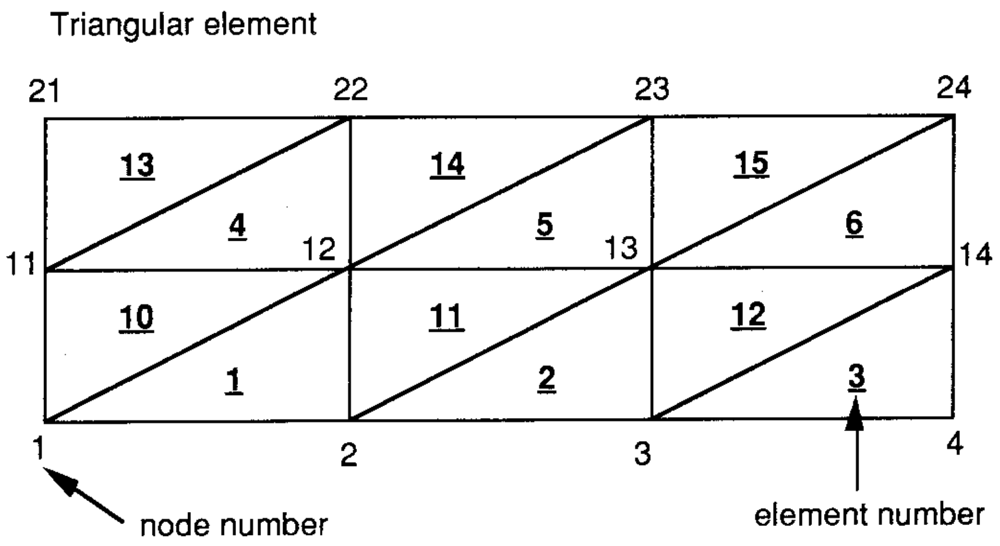
12. Element Data for Composite Element

Header Card

Column	entry	contents	format
1 ~ 4	'ELEM'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'ELEM'		A4
11 ~ 15	K1	element number	I5
16 ~ 20	K2	1-st node number of the element	I5
21 ~ 25	K3	2-nd node number of the element	I5
26 ~ 30	K4	3-rd node number of the element	I5
31 ~ 35	K5	4-th node number of the element	I5
36 ~ 38	K6	hydraulic conductivity No.	I3
39 ~ 41	K7	function No. of hydraulic property	I3
42 ~ 44	K8	condition No. of water flux (<100 : related to SOUR card, >100 : related to user-routine SORUSE)	I3
46 ~ 55	R1	porosity of the material	F10.0
67 ~ 68	L1	flag of automatic generation of element =0:square element =1:triangular element (L3:generate I-K direction) =2:triangular element (L3:generate J-K direction)	I2
69 ~ 70	L2	number of generating element (I-J direction)	I2
71 ~ 72	L3	number of generating element (I-L direction)	I2



```
                                        L1  L2  L3
ELEM    1    1    2   12    0 ...... 2   3   2
ELEM   10   11    1   12    0 ...... 1   2   3
```

Fig. A-3 Triangular element of composite element

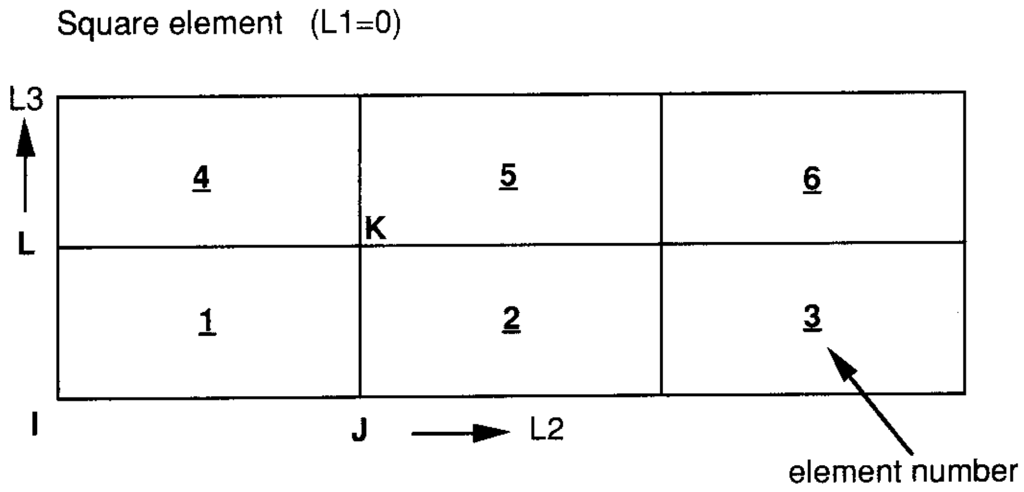


Fig. A-4 Square element of composite element

13. Isoparametric Element

Header Card

Column	entry	contents	format
1 ~ 4	'ISOE'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'ISOE'		A4
11 ~ 15	K1	element number	I5
16 ~ 20	I1	1-st node number of this element	I5
21 ~ 25	I2	2-nd node number of this element	I5
26 ~ 30	I3	3-rd node number of this element	I5
31 ~ 35	I4	4-th node number of this element	I5
36 ~ 40	I5	5-th node number of this element	I5
41 ~ 45	I6	6-th node number of this element	I5
46 ~ 50	I7	7-th node number of this element	I5
51 ~ 55	I8	8-th node number of this element	I5
61 ~ 63	KN	hydraulic conductivity number	I3
64 ~ 66	KF	function No. of hydraulic property	I3
67 ~ 68	L1	=0:square element, =1:triangular element	I2
69 ~ 70	L2	number of generating element (I1-I2 direction)	I2
71 ~ 72	L3	number of generating element (I1-I4 direction)	I2

2-nd Card

Column	entry	contents	format
1 ~ 4	' '	2nd card of ISOE data	A4
11 ~ 20	R1	porosity of the material	F10.0
21 ~ 25	L1	condition No. of water flux (blank:no flux), related to SOUR card(<100) and user-routine SORUSE (>100)	I5
26 ~ 30	L2	condition No. of nuclide flux (blank:no flux), related to NSET and CPRO cards	I5
31 ~ 35	L3	condition No. of the material (related to MAT1 card)	I5
36 ~ 40	L4	condition No. of the material (related to NSET and MAT2 cards)	I5

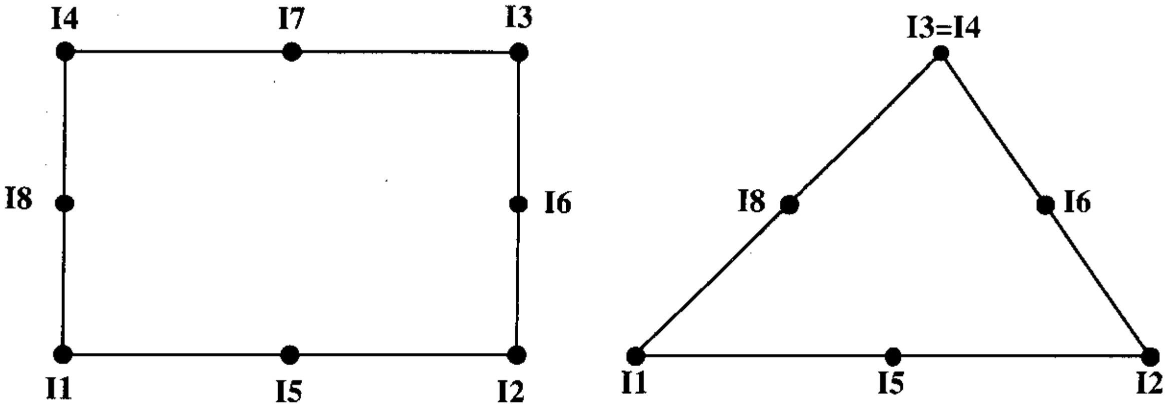


Fig. A-5 Isoparametric elements (triangular element : I3 and I4 are degenerated)

14. Boundary Data for Composite Elements

Header Card

Column	entry	contents	format
1 ~ 4	'BOUN'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'BOUN'		A4
11 ~ 15	K1	node number of the boundary	I5
16 ~ 20	K2	node number of the boundary	I5
21 ~ 25	LQR	condition No. of rainfall recharge (related to RAIN card)	I5
26 ~ 35	QR	rainfall recharge (steady state)	F10.0
36 ~ 40	LQF	condition No. of normal velocity (related to VELO card)	I5
41 ~ 50	QF	normal velocity (steady state)	F10.0
76 ~ 80	MM	increment of node number for automatic generation (MM=blank:no automatic generation)	I5

2-nd Card

Column	entry	contents	format
1 ~ 4	'BOUN'	2nd card of BOUN data for automatic generation	A4
11 ~ 15	K1	node number of the boundary	I5
16 ~ 20	K2	node number of the boundary	I5

15. Boundary Data for Isoparametric Element

Header Card

Column	entry	contents	format
1 ~ 4	'ISOB'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'ISOB'		A4
11 ~ 15	K1	node number of the boundary	I5
16 ~ 20	K2	node number of the boundary	I5
21 ~ 25	K3	node number of the boundary	I5
31 ~ 35	LQR	condition No. of rainfall recharge (related to RAIN card)	I5
36 ~ 40	LQF	condition No. of normal velocity (related to VELO card)	I5
41 ~ 45	LQN	condition No. of nuclide flux (related to NSET and FLUX cards)	I5
76 ~ 80	MM	increment of node number for automatic generation (MM=blank:no automatic generation)	I5

2-nd Card

Column	entry	contents	format
1 ~ 4	'ISOB'	2nd card of ISOB data for automatic generation	A4
11 ~ 15	K1	node number of the boundary	I5
16 ~ 20	K2	node number of the boundary	I5
21 ~ 25	K3	node number of the boundary	I5

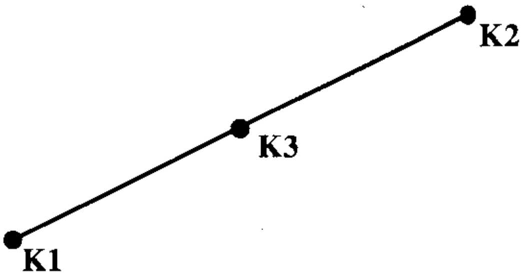


Fig. A-6 Boundary data for isoparametric element

16. Water Level Data for Groundwater Flow Analysis

Header Card

Column	entry	contents	format
1 ~ 4	'LINE'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'LINE'		A4
11 ~ 15	K1	index of water level data	I5
21 ~ 25	K2	number of nodes composing a water level-line	I5
26 ~ 30	K3	condition No. of water level (only for transient state) water level must be inputted by HEAD card	I5
31 ~ 40	HIGH	water level for steady state	F10.0

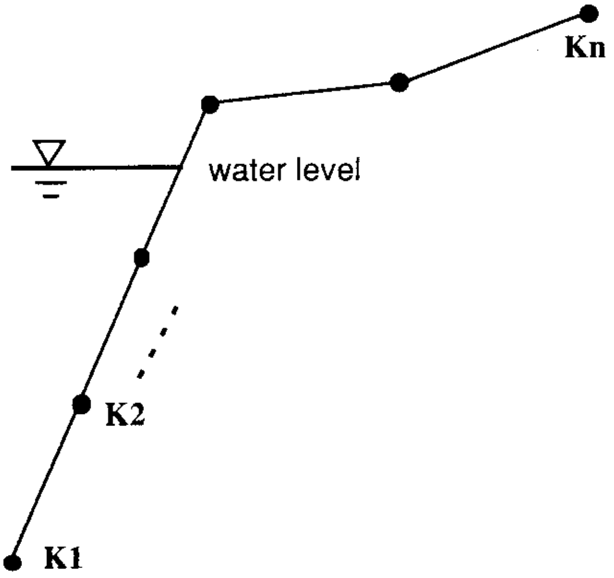


Fig. A-7 Water level data

2-nd Card

Column	entry	contents	format
1 ~ 4	'LINE'		A4
21 ~ 70	K1 ~Kn	node numbers composing a water level-line if n>10, similar card is necessary	10I5

3-rd Card

Column	entry	contents	format
1 ~ 4	'LINE'		A4
11 ~ 15	N1	index of water level data	I5
21 ~ 25	N2	number of nodes composing a water level-line	I5
26 ~ 30	N3	condition No. of water level (only for transient state) water level must be inputted by HEAD card	I5
31 ~ 40	HIGH	water level for steady state	F10.0
41 ~ 45	K1	initial node number composing a water level-line	I5
46 ~ 50	Kn	final node number composing a water level-line	I5
69 ~ 72	NN	increment of node number (K1~Kn :sequential)	I4

17. Setting of Analytic Conditions for Nuclide Transport

These data specify the boundary conditions for nuclide transport analysis and material data concerning to nuclide transport.

Header Card

Column	entry	contents	format
1 ~ 4	'NSET'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'NSET'		A4
11 ~ 15	N	condition No. for nuclide transport analysis, N corresponds to K1 and K2 in the NODE card, L2, L3 and L4 in the 2nd card of ISOE data	
16 ~ 65	K1 ~Kn	K1:condition No. for 1-st nuclide, Kn:condition No. for n-th nuclide, These values indicate nuclide flux from node, element and boundary (CPRO and FLUX card), concentrations of nodes (FCNC card) and material properties (MAT2 card). if Kn<0:user-routines(CNCSET,FGENER,CGENER)	10I5

18. Rainfall Recharge Data for the boundary

Header Card

Column	entry	contents	format
1 ~ 4	'RAIN'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'RAIN'		A4
11 ~ 15	KK	condition No. (LQR of BOUN and ISOB data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'RAIN'		A4
21 ~ 70	R(1) ~R(N)	R(1):rainfall recharge corresponds to time T(1), R(N):rainfall recharge corresponds to time T(N)	10F5.0

19. Hydraulic Head Data

Header Card

Column	entry	contents	format
1 ~ 4	'HEAD'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'HEAD'		A4
11 ~ 15	KK	condition No. (L2 of NODE and N3 of LINE data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'HEAD'		A4
21 ~ 70	R(1) ~R(N)	R(1):water level corresponds to time T(1), R(N):water level corresponds to time T(N)	10F5.0

20. Normal Velocity Data for the Boundary

Header Card

Column	entry	contents	format
1 ~ 4	'VELO'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'VELO'		A4
11 ~ 15	KK	condition No. (LQF of BOUN and ISOB data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2nd Card

Column	entry	contents	format
1 ~ 4	'VELO'		A4
21 ~ 70	R(1) ~R(N)	R(1):normal velocity corresponds to time T(1), R(N):normal velocity corresponds to time T(N)	10F5.0

21. Water Fluxes from Nodes and Elements

Header Card

Column	entry	contents	format
1 ~ 4	'SOUR'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'SOUR'		A4
11 ~ 15	KK	condition No. (L1 of NODE, K8 of ELEM and L1 of ISOE data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'SOUR'		A4
21 ~ 70	R(1) ~R(N)	R(1):water flux corresponds to time T(1), R(N):water flux corresponds to time T(N)	10F5.0

22. Nuclide Concentration Data for Boundary Condition

Header Card

Column	entry	contents	format
1 ~ 4	'FCNC'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'FCNC'		A4
11 ~ 15	KK	condition No. (K2 of NODE data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'FCNC'		A4
21 ~ 70	R(1) ~R(N)	R(1):nuclide concentration corresponds to time T(1), R(N):nuclide concentration corresponds to time T(N)	10F5.0

23. Nuclide Flux from the Boundary

Header Card

Column	entry	contents	format
1 ~ 4	'FLUX'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'FLUX'		A4
11 ~ 15	KK	condition No. (LQN of ISOB data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'FLUX'		A4
21 ~ 70	R(1) ~R(N)	R(1):nuclide flux from boundary corresponds to time T(1), R(N):nuclide flux from boundary corresponds to time T(N)	10F5.0

24. Nuclide Fluxes from Nodes and Elements

Header Card

Column	entry	contents	format
1 ~ 4	'CPRO'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'CPRO'		A4
11 ~ 15	KK	condition No. (K1 of NODE and L2 of ISOE data)	I5
16 ~ 20	N	number of dividing simulative time (N<11)	I5
21 ~ 70	T(1) ~T(N)	T(1):1-st time, T(N):N-th time	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'CPRO'		A4
21 ~ 70	R(1) ~R(N)	R(1):nuclide flux from node and element corresponds to time T(1), R(N):nuclide flux from node and element corresponds to time T(N)	10F5.0

25. Hydraulic Conductivity Data

Column	entry	contents	format
1 ~ 4	'COND'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'COND'		A4
11 ~ 15	K1	index (K6 of ELEM and KN of ISOE data)	I5
21 ~ 30	Kxx	XX-component of hydraulic conductivity	F10.0
31 ~ 40	Kxy	XY-component of hydraulic conductivity	F10.0
41 ~ 50	Kyy	YY-component of hydraulic conductivity	F10.0
51 ~ 60	CR	compressibility of material	F10.0

26. Hydraulic Property Data

Header Card

Column	entry	contents	format
1 ~ 4	'C.CO'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'TH-H'		A4
11 ~ 15	KK	function No. (K7 of ELEM and KF of ISOE data)	I5
16 ~ 20	N	number of dividing hydraulic property curve (N<11)	I5
21 ~ 70	TH(1) ~TH(N)	TH(1):water content of 1-st point, TH(N):water content of N-th point	10F5.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'TH-H'		A4
21 ~ 70	HP(1) ~HP(N)	HP(1):pressure head corresponds to TH(1), HP(N):pressure head corresponds to TH(N)	10F5.0

3-rd Card

Column	entry	contents	format
1 ~ 4	'TH-K'		A4
16 ~ 20	N	number of dividing hydraulic property curve (N<11)	I5
21 ~ 70	TH(1) ~TH(N)	TH(1):water content of 1-st point, TH(N):water content of N-th point	10F5.0

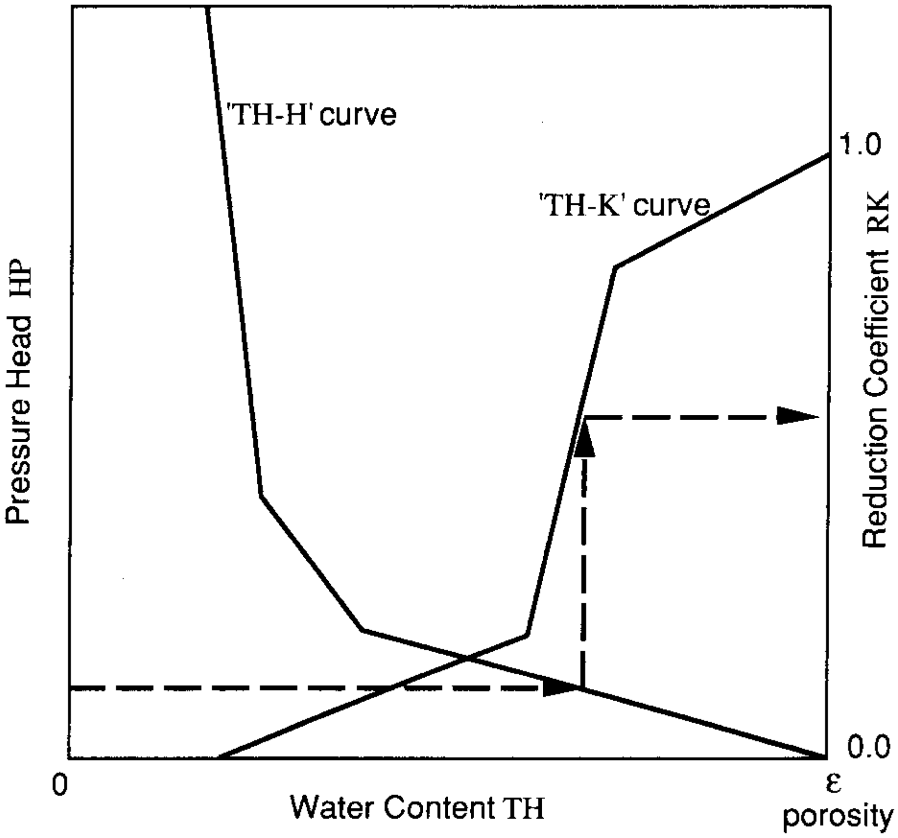


Fig. A-8 Hydraulic property curve

4-th Card

Column	entry	contents	format
1 ~ 4	'TH-K'		A4
21 ~ 70	RK(1) ~RK(N)	RK(1):reduction coefficient corresponds to TH(1), RK(N):reduction coefficient corresponds to TH(N)	10F5.0

5-th Card

Column	entry	contents	format
1 ~ 4	'VEL-'		A4
16 ~ 20	N	number of dividing hydraulic property curve (N<11)	I5
21 ~ 70	V(1) ~V(N)	V(1):water velocity of 1-st point, V(N):water velocity of N-th point	10F5.0

6-th Card

Column	entry	contents	format
1 ~ 4	'VEL-'		A4
21 ~ 70	RK(1) ~RK(N)	RK(1):reduction coefficient corresponds to V(1), RK(N):reduction coefficient corresponds to V(N)	10F5.0

27. Material Data for Nuclide Transport

Header Card of MAT1 Data

Column	entry	contents	format
1 ~ 4	'MAT1'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'MAT1'		A4
11 ~ 15	K1	index (L3 of ISOE data)	I5
21 ~ 30	DL	longitudinal dispersion length	F10.0
31 ~ 40	DT	transverse dispersion length	F10.0
41 ~ 50	DD	molecular diffusion coefficient	F10.0
51 ~ 60	TA	tortuosity	F10.0

Header Card of MAT2 Data

Column	entry	contents	format
1 ~ 4	'MAT2'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'MAT2'		A4
11 ~ 15	K1	index (L4 of ISOE data)	I5
21 ~ 30	RD	retardation factor of nuclide	F10.0
31 ~ 40	DU1	dummy =0.0	F10.0
41 ~ 50	DU2	dummy =0.0	F10.0

28. Nuclide Data

Header Card

Column	entry	contents	format
1 ~ 4	'NUCL'	Header card	A4
5 ~ 80	blank		

1-st Card

Column	entry	contents	format
1 ~ 4	'NUCL'		A4
9 ~ 10	II	index of nuclide	I2
11 ~ 30	NN	name of nuclide	5A4
31 ~ 40	RR	decay constant of nuclide	F10.0

2-nd Card

Column	entry	contents	format
1 ~ 4	'NUCL'		A4
11 ~ 20	R1	transfer rate from i-th nuclide to i+1-th nuclide $\xi_{i+1,i}$	F10.0
21 ~ 30	R2	transfer rate from i-th nuclide to i+2-th nuclide $\xi_{i+2,i}$	F10.0
31 ~ 40	R3	transfer rate from i-th nuclide to i+3-th nuclide $\xi_{i+3,i}$	F10.0
41 ~ 50	R4	transfer rate from i-th nuclide to i+4-th nuclide $\xi_{i+4,i}$	F10.0

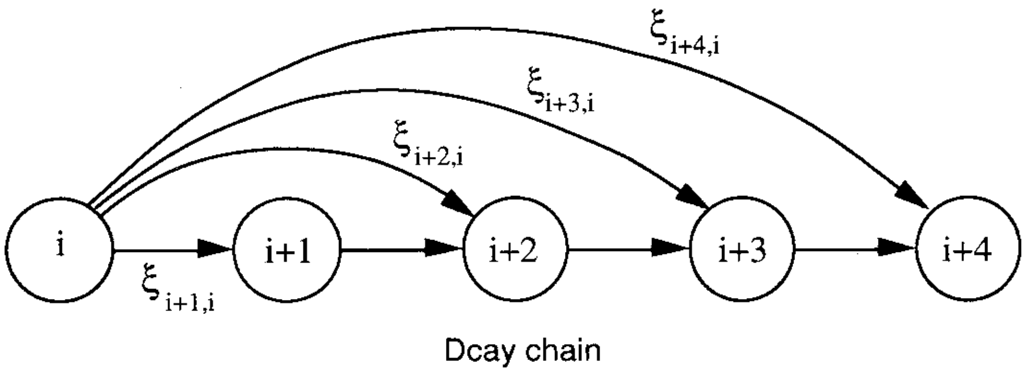


Fig. A-9 Treatment of radioactive dcay

29. Initial Condition of Pressure Head

Column	entry	contents	format
1 ~ 4	'INIT'		A4
11 ~ 15	N	node number to be initialized (initial node number)	I5
16 ~ 25	RR	initial pressure head	F10.0
26 ~ 30	M	final node number for automatic generation	I5
31 ~ 35	L	increment of node number for automatic generation	I5

30. Initial Condition of Temperature

Column	entry	contents	format
1 ~ 4	'TEMP'		A4
11 ~ 15	N	node number to be initialized (initial node number)	I5
16 ~ 25	RR	initial temperature	F10.0
26 ~ 30	M	final node number for automatic generation	I5
31 ~ 35	L	increment of node number for automatic generation	I5

31. Initial Condition of Nuclide Concentration

Column	entry	contents	format
1 ~ 4	'CONC'		A4
9 ~ 10	II	index No. of nuclide	I2
11 ~ 15	N	node number to be initialized (initial node number)	I5
16 ~ 25	RR	initial concentration of nuclide	F10.0
26 ~ 30	M	final node number for automatic generation	I5
31 ~ 35	L	increment of node number for automatic generation	I5

32. End Date of Job

Column	entry	contents	format
1 ~ 4	'END'		A4
5 ~ 80	blank		

II. Input Data for Plotting Results

1. Job Identification Card for figures of mesh, vectors and contours

Column	entry	contents	format
1 ~ 4	'STEP'		A4
11 ~ 18		enter 'PLOTSEEP'	2A4

2.Title Card

Column	entry	contents	format
1 ~ 4	'TITL'		A4
11 ~ 74		enter 'Title name'	16A4

3. Plot Data Card for Groundwater Flow

Column	entry	contents	format
1 ~ 8	'PLOTSEEP'		2A4
11	L1	=1:plot mesh figure	I1
12	L2	=1:plot steady results	I1
13	L3	=1:plot transient results	I1
16 ~ 20	L4	initial No. of time step for plotting	I5
21 ~ 25	L5	final No. of time step for plotting	I5
26 ~ 30	L6	increment of time step for plotting	I5
36	M1	=1:plot mesh only	I1
37	M2	=1:plot mesh + element No.	I1
38	M3	=1:plot mesh + node No.	I1
39	M4	=1:plot mesh + element No. + node No.	I1
41	N1	=1:plot contour of pressure head, =2:plot contour of total head, =3:plot contour of dynamic pressure	I1
42	N2	=1:plot water table	I1
43	N3	=1:plot velocity vector	I1
44	N4	=1:plot water table + velocity vector	I1
45	N5	=1:plot contour of pressure head+velocity vector =2:plot contour of total head+velocity vector =3:plot contour of dynamic pressure+ velocity vector	I1
49 ~ 50	KK	frame size of plotting area (A4,A3,A2,A1,A0,B4,B3,B2,B1)	A2
51 ~ 55	RX	distance in the X-direction between frame and bottom of the left side of the figure	F5.0
56 ~ 60	RY	distance in the Y-direction between frame and bottom of the left side of the figure	F5.0

4. Plot Data Card for Nuclide Transport

Column	entry	contents	format
1 ~ 8	'PLOTNUCL'		2A4
11	L1	=1:plot mesh figure	I1
13	L3	=1:plot contour of concentration	I1
16 ~ 20	L4	initial No. of time step for plotting	I5
21 ~ 25	L5	final No. of time step for plotting	I5
26 ~ 30	L6	increment of time step for plotting	I5
36	M1	=1:plot mesh only	I1
37	M2	=1:plot mesh + element No.	I1
38	M3	=1:plot mesh + node No.	I1
39	M4	=1:plot mesh + element No. + node No.	I1
41	N1	=1:plot contour of 1-st nuclide	I1
42	N2	=1:plot contour of 2-nd nuclide	I1
43	N3	=1:plot contour of 3-rd nuclide	I1
44	N4	=1:plot contour of 4-th nuclide	I1
45	N5	=1:plot contour of 5-th nuclide	I1
49 ~ 50	KK	frame size of plotting area (A4,A3,A2,A1,A0,B4,B3,B2,B1)	A2
51 ~ 55	RX	distance in the X-direction between frame and bottom of the left side of the figure	F5.0
56 ~ 60	RY	distance in the Y-direction between frame and bottom of the left side of the figure	F5.0

5. Scale Card (scaling of plotting)

Column	entry	contents	format
1 ~ 4	'SCAL'		A4
11 ~ 20	R1	plot scale of X-direction (size=X*R1 mm)	F10.0
21 ~ 30	R2	plot scale of Y-direction (size=Y*R2 mm)	F10.0
31 ~ 40	R3	plot scale of velocity (size=V*R3 mm)	F10.0
41 ~ 50	R4	interval of contour line	F10.0

6.End Card

Column	entry	contents	format
1 ~ 4	'END'		A4
5 ~ 80	blank		

1. Job Identification Card for Plotting of History Data

Column	entry	contents	format
1 ~ 4	'STEP'		A4
11 ~ 18		enter 'HISTORY'	2A4

2. Title Card

Column	entry	contents	format
1 ~ 4	'TITL'		A4
11 ~ 74		enter 'Title name'	16A4

3. Plot Data Card for Groundwater Flow

Column	entry	contents	format
1 ~ 8	'HISTSEEP'		2A4
11 ~ 15	I1	number of elements to be printed out their histories of velocity	I5
16 ~ 40	K1 ~K5	element No.	5I5
46 ~ 50	IT1	number of nodes to be printed out their histories of temperature	I5
51 ~ 75	KT1 ~KT5	node No.	5I5

4. Plot Data Card for Nuclide Transport

Column	entry	contents	format
1 ~ 8	'HISTNUCL'		2A4
46 ~ 50	N	number of nodes to be printed out their histories of concentration	I5
51 ~ 75	L1 ~L5	node No.	5I5

5. Plot Data (plot items)

Column	entry	contents	format
1 ~ 4	'PLOT'		A4
11 ~ 15	N1	number of figures (velocity or temperature)	I5
16 ~ 55	I1 ~I8	=11:X-component of velocity Vx =12:Y-component of velocity Vy =13:absolute value of velocity |V| =21:Vx and Vy =31:Vx, Vy and |V| =-11:temperature	8I5
56 ~ 60	K1	initial time step of plotting	I5
61 ~ 65	K2	final time step of plotting	I5

6. Plot Data (nuclide)

Column	entry	contents	format
1 ~ 4	'PLOT'		A4
11 ~ 15	N	number of nuclides for plotting	I5
16 ~ 40	I1 ~I5	nuclide No.	5I5

7. Scale Card

Column	entry	contents	format
1 ~ 4	'SCAL'		A4
11 ~ 20	R1	standard value of time-axis	F10.0
21 ~ 30	R2	maximum value of time-axis	F10.0
31 ~ 40	R3	standard value of velocity	F10.0
41 ~ 50	R4	maximum value of velocity	F10.0
51 ~ 60	R5	standard value of temperature or concentration	F10.0
61 ~70	R6	maximum value of temperature or concentration	F10.0

8. End Card

Column	entry	contents	format
1 ~ 4	'END'		A4
5 ~ 80	blank		

Appendix 2 Restart runs and data files

This code has a function of restart run to save the computational sizes. Flow of restart runs and necessary files for the computation are shown in Fig. A-10.

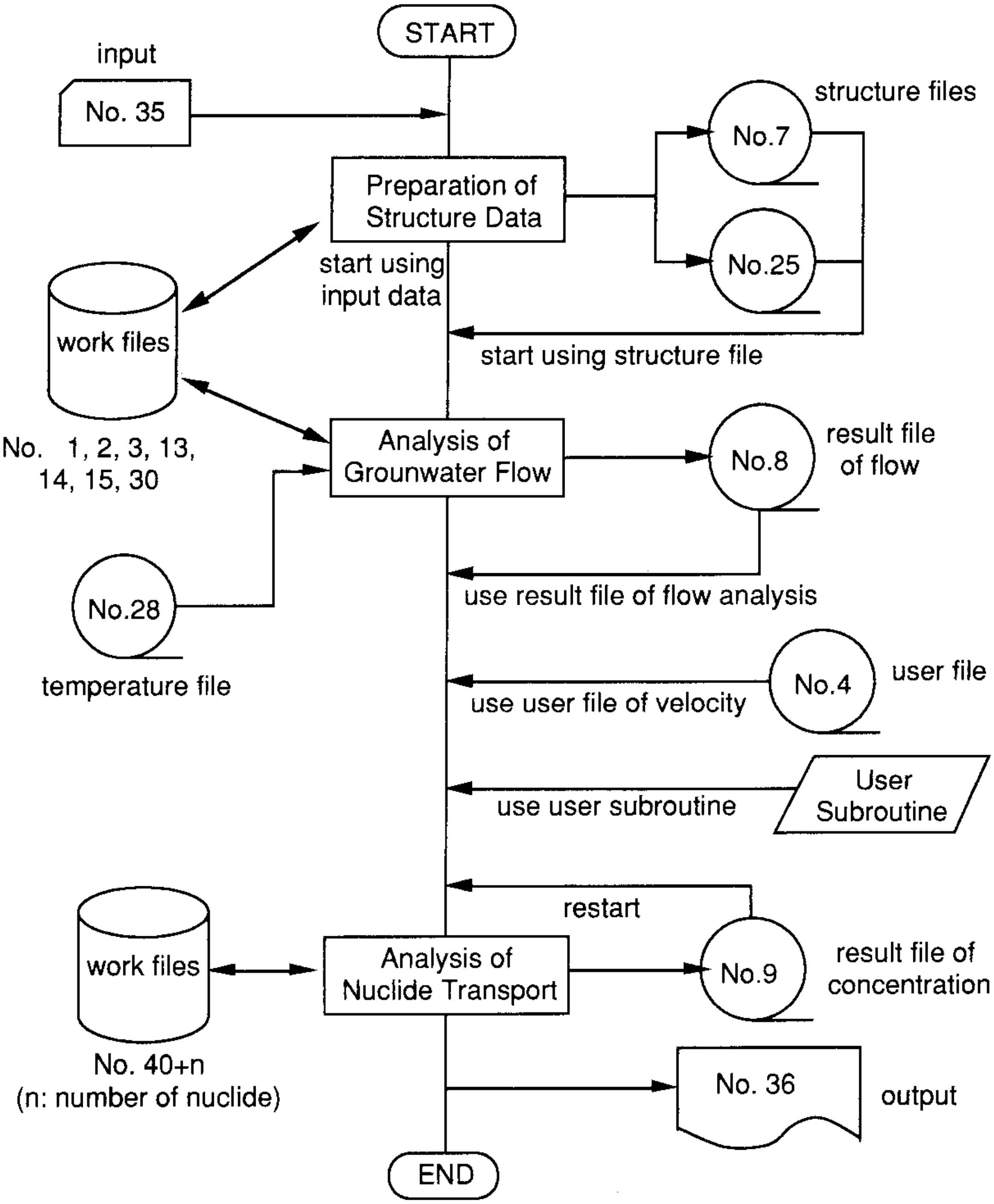


Fig. A-10 Flow of restart runs and necessary files

Appendix 3 User subroutines

The following subroutines are prepared for the computations with this code.

1. 'FLOWB' : defines relative fluid density $\rho(T)/\rho_0$
input arguments T : temperature
IMAT : dummy
IFLG : dummy
ITO : file No. of output
ICK : debug parameter
output argument BHAT : $\rho(T)/\rho_0$

2. 'SORUSE' : defines source strength of water flux from element
input arguments INDEX : condition No. of water flux (> 100)
(K8 of ELEM card and L1 of ISOE card)
TIME : time
output argument VALUE : source strength

3. 'VISCOS' : defines relative fluid viscosity $\mu(T)/\mu_0$
input arguments NO : function No. of viscosity
(I1 of WATE card)
TEMP : temperature
ITO : file No. of output
ICK : debug parameter
output argument G : $\mu(T)/\mu_0$

4. 'CNCSET' : defines boundary conditions for concentrations of radionuclides
input arguments NO : condition No. of the concentration (< 0)
(Kn of NSET card)
T : time
ITO : file No. of output
ICK : debug parameter
output argument CX : the concentration of radionuclide

5. 'FGENER' : defines nuclide fluxes from boundaries
input arguments NO : condition No. of nuclide flux (< 0)
(Kn of NSET card)

$-2000 < NO < -999$: $q = \mathbf{n}\,(\mathbf{u}C - \mathbf{D}\mathrm{grad}C)$
$-3000 < NO < -1999$: $q = -\mathbf{n}\,\mathbf{D}\mathrm{grad}C$
$-4000 < NO < -2999$: $q = -\mathbf{n}\,\mathrm{grad}C$
T : time
ITO : file No. of output
ICK : debug parameter
output argument CX : the flux of radionuclide

6. 'CGENER' : defines nuclide fluxes from nodes and elements
input arguments NO : condition No. of the nuclide flux (< 0) (Kn of NSET card)
T : time
ITO : file No. of output
ICK : debug parameter
output argument CX : the flux of radionuclide

7. 'VELOC' : defines the Darcy's velocities of the domain
This subroutine will be called when 'I4' of CONT card is '63' or '66'.
input arguments X : x-coordinate
Y : y-coordinate
ITO : file No. of output
ICK : debug parameter
output arguments UX : x-component of the Darcy's velocity
UY : y-component of the Darcy's velocity

Appendix 4 Extension of program-size

The program-size must be changed according to the size of numerical analysis. The following variables must be changed to appropriate values.

1. Total size of work area : IW(******), IW(1) of main program
2. Maximum number of node : MEE(67) of subroutine 'COMSET'
3. Maximum number of element : MEE(68) of subroutine 'COMSET'
4. Maximum number of boundary data : MEE(69) of subroutine 'COMSET'
5. Maximum number of LINE data : MEE(70) of subroutine 'COMSET'
6. Maximum number of water flux data : MEE(71) of subroutine 'COMSET'
7. Maximum number of rainfall recharge : MEE(72) of subroutine 'COMSET'
8. Maximum number of normal velocity : MEE(73) of subroutine 'COMSET'
9. Maximum number of HEAD data : MEE(74) of subroutine 'COMSET'
10. Maximum number of hydraulic conductivity data : MEE(75) of subroutine 'COMSET'
11. Maximum number of hydraulic property data : MEE(76) of subroutine 'COMSET'
12. Maximum number of time step : MEE(77) of subroutine 'COMSET'
13. Size of matrix data (size of work area) : MEE(79) of subroutine 'COMSET'
14. Maximum number of nodes constructing LINE data : MJOINT of subroutine 'COMSET'