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COMPUTER CODE TRANS-ACE PREDICTING FOR FIRE AND EXPLOSION ACCIDENTS IN NUCLEAR FUEL REPROCESSING PLANTS

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Computer Code TRANS-ACE Predicting for Fire and Explosion Accidents in Nuclear Fuel Reprocessing Plants

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(Received October 12, 1993)

The accident analysis code TRANS-ACE was developed to evaluate the safety of a ventilation system in a reprocessing plant in the event of fire and explosion accidents. TRANS-ACE can evaluate not only the integrity of a ventilation system containing HEPA filters but also the source term of radioactive materials for release out of a plant. It calculates the temperature, pressure, flow rate, transport of combustion materials and confinement of radioactive materials in the network of a ventilation system that might experience a fire or explosion accident.

TRANS-ACE is based on the one-dimensional compressible thermo-fluid analysis code EVENT developed by Los Alamos National Laboratory (LANL). Calculational functions are added for the radioactive source term, heat transfer and radiation to cell and duct walls and HEPA filter integrity.

For the second edition in the report, TRANS-ACE has been improved incorporating functions for the initial steady-state calculation to determine the flow rates, pressure drops and temperature in the network before an accident mode analysis. It is also improved to include flow resistance calculations of the filters and blowers in the network and to have an easy to use code by simplifying the input formats.

This report is to prepare an explanation of the mathematical model for TRANS-ACE code and to be the user's manual.

Keywords: TRANS-ACE, Computer Code, Safety, Reprocessing Plants, Fire, Explosion, Smoke, Radioactive Materials, Transport, Compressible Thermo-fluid Analysis, Aerosol, HEPA Filter

再処理施設における火災及び爆発事故解析コード TRANS－ACE の開発

日本原子力研究所東海研究所燃料サイクル安全工学部
阿部　仁・西尾　軍治・内藤　俶孝

（1993 年 10 月 12 日受理）

再処理施設の事故時安全性を評価する目的で事故解析コード TRANS－ACE の開発を進めている。TRANS－ACE は再処理施設内での溶媒火災と爆発事故を対象として，事故発生からセル換気系内温度・圧力伝播，放射性物質移行解析，HEPA フィルタによる放射性物質の捕集解析等を行い，施設の健全性評価と最終的な施設外への放射性物質の放出までを一貫して計算する。

TRANS－ACE は米国ロスアラモス国立研究所で開発された 1 次元熱流動解析コード EVENT をベースに，溶媒火災事故時の燃焼・鎮火モデル，爆発事故解析モデル等ソースターム解析機能，セルやダクト壁面への放熱計算機能さらに HEPA フィルタ捕集解析機能等を付加し作成された。

今回既に作成した TRANS－ACE に，流量による収束判定機能の追加（初期定常状態設定時），フィルタ・ブロアの流動抵抗自動計算機能の追加，入力データ形式の整理，簡素化の 3 点について改良を加え TRANS－ACE の 2 次版を作成した。

本報告書はコードの使用手引書であると同時に解析機能説明書である。

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

It is important to evaluate the integrity of HEPA filters and the confinement of radioactive materials in a ventilation system of a fuel reprocessing plant under the possible condition of an accident. Under this view, the computer code TRANS-ACE for the safety evaluation in the event of a fire or explosion in a plant has been developed at JAERI[1]. TRANS-ACE can calculate the source term of radioactive materials under fire and explosion conditions and confinement of radioactivities in the ventilation system.

EVENT, developed in Los Alamos National Laboratory (LANL)[2], is an explosion analysis code for one-dimensional compressible thermo-fluid behavior in nuclear fuel cycle facilities, but it is not programmed to calculate the behavior of aerosol containing radioactive materials. Furthermore, EVENT is not programmed to calculate the heat transfer to the wall of cells and ducts in a ventilation system. TRANS-ACE is based on EVENT code and developed by adding a solvent pool burning model, fire extinction model, explosion model involving heat and mass transfer and high efficiency particle air (HEPA) filter model containing a smoke behavior model. Automatic calculations of the flow resistance of cells, valves, filters and blowers in the ventilation system are provided by input data of shapes and length of the ventilation system. Volume flow through the ventilation system is also calculated automatically with the opening and closing movements of a check valve at the inlet of cells.

In addition, it has been improved to advance calculation functions of the previous version of TRANS-ACE in the following way:

(1) The judgment of iteration convergence at the initial steady-state calculation is added by the adjustment of flow rate determined in the ventilation.

(2) Automatic calculation of flow resistance for filters and blowers is added.

(3) Arrangement and simplification of input data are provided to use the code conveniently.

This document is divided to seven chapters. When the user does not need any detailed information regarding TRANS-ACE, Chapter 3 (Functions of initial steady-state calculation) and Chapter 4 (Functions of accident calculation) need not be read.

2. OUTLINE OF TRANS-ACE

2.1 Outline of calculational functions in the code

Figure 2.1 shows a system flow chart for TRANS-ACE. The user will be able to utilize the TRANS-ACE code by selecting combinations of many functions with calculational flags set in TRANS-ACE as shown in Chapter 5. TRANS-ACE has also a restart system in the middle of the calculation.

Figure 2.2 shows the relationship among these functions in TRANS-ACE, consisting of a source-term calculation concerning fire and explosion, one-dimensional thermo-fluid calculation and transport calculation of aerosol containing radioactive materials. TRANS-ACE also can calculate mass and heat transfers, heat conduction to the cell and duct walls in the ventilation system and transport from the accidental source passing through HEPA filters to the environment during fire and explosion accidents.

The source-term calculation consists of two: one is directly given by users as input for the variations in pressure and temperature, mass and energy release and aerosol release during a fire or explosion, another by inner calculational models programmed in the code. The modified Spalding's B-factor model[3)4)] is used for the calculation of the solvent burning in TRANS-ACE as a function of the burning area and airflow rate into a fire cell, involving an extinction model. On the other hand, EVENT'84 model[5)] in LANL is used for the calculation of an explosion.

Figure 2.3 shows flow chart of TRANS-ACE consisting of an initial steady-state calculation and accident calculation. Initial conditions of the flow rate, pressure difference and temperature in the ventilation system must be set before the calculation of accidents. In the accident calculation, temperature, pressure, flow rate of thermo-fluid and aerosol containing radioactive materials in the ventilation system can be calculated with the values of initial steady-state calculation.

TRANS-ACE has some adding functions for preparation of input data and realization of a practical calculation model.

(1) Automatic calculation of flow resistance in a ventilation system

Resistances of the ducts, valves, filters and blowers are calculated from values of their shape and size with given flow rates in the ventilation system by using the initial steady-state calculation of TRANS-ACE.

(2) Automatic calculation of openning and shutting of the valve

This function is the flow rate control calculation for automatic valve openning and shutting by monitoring flow rate and pressure at the node point in the ventilation system.

(3) Function of automatically set check valves at the inlet of cells

Check valves are equipped in the reprocessing plant between the cell and environment of the plant, so that TRANS-ACE has a calculational function to automatically set check valves at the boundary points between the cell and environment.

(4) Function of the automatic time step

Two functions are set in TRANS-ACE for time step. One is given by input as time step data by the user, and the other is by the automatic time step in the code by using time variation of the mass and energy release rates. In large mass and energy release rates such as a big explosion, the a time step will be required to provide a much shorter time step.

2.2 Calculation of the node-junction method

TRANS-ACE was based on the one-dimensional compressible thermofluid analysis code of EVENT developed in LANL[2] using the calculation of the node-junction method. The ventilation system is divided into several volume elements as nodes for calculating pressures, densities and temperatures, and several resistance elements as branches for calculating volume flows in the node junction method. This method is very useful for thermo-fluid analysis applied to a complex network in a reprocessing plant. Figure 2.4 shows a sample of node-junction of the ventilation

system.

The definition of the node-junction is expressed as follows:

System: This is a network of duct components as branches joined with a cell called the node.

Node: This is a volume element which is volume capacitance connected among one or more branches, such as a cell, room, glovebox and plenum. Some volume elements are set up as a node in middle of the duct. Compressibility of the fluid is calculated in the volume capacitance of the node. Boundary points between the cell and environment also are specified as nodes in TRANS-ACE. Number of nodes can be set up to 210 which are 200 volume nodes and 10 boundary points.

Branch: This is the flow resistance element such as the duct between upstream and downstream nodes. The branch corresponds to the duct, valve, damper, filter and blower in the ventilation system. Flow rate is calculated by the flow resistance in these branches. Number of branches is set up to 200 in the ventilation system.

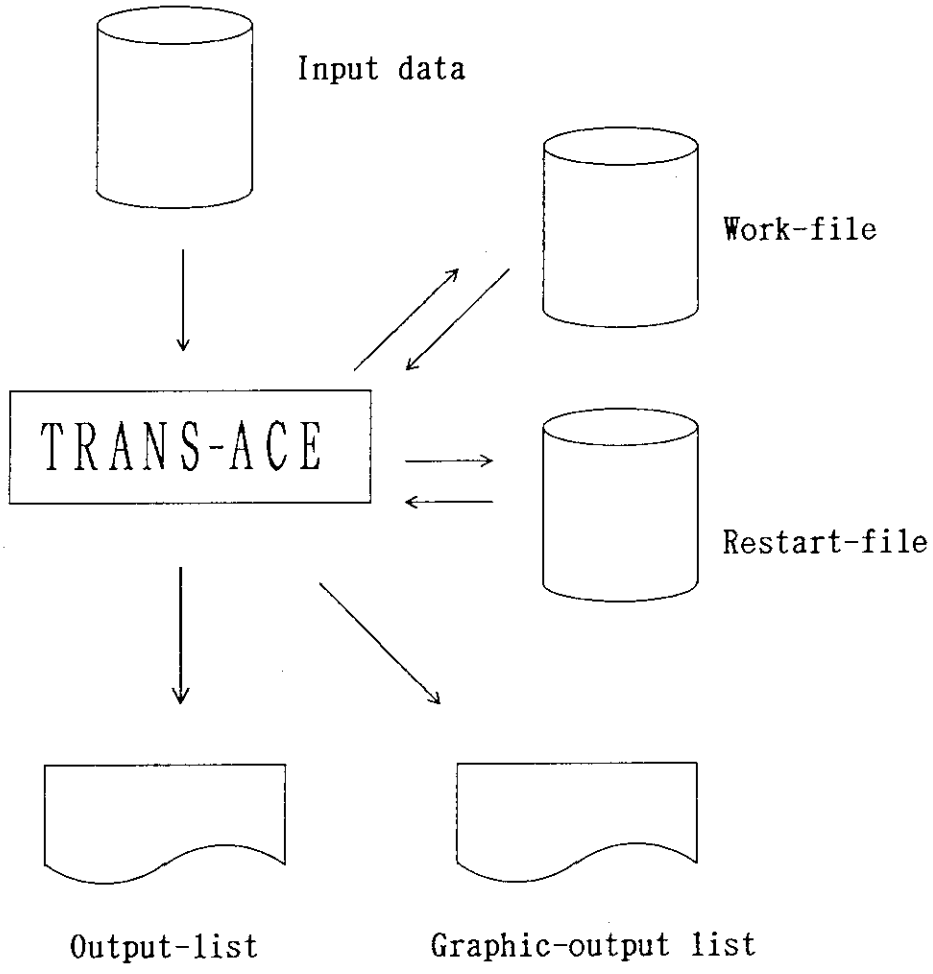

Fig. 2.1 System flow chart of TRANS－ACE.

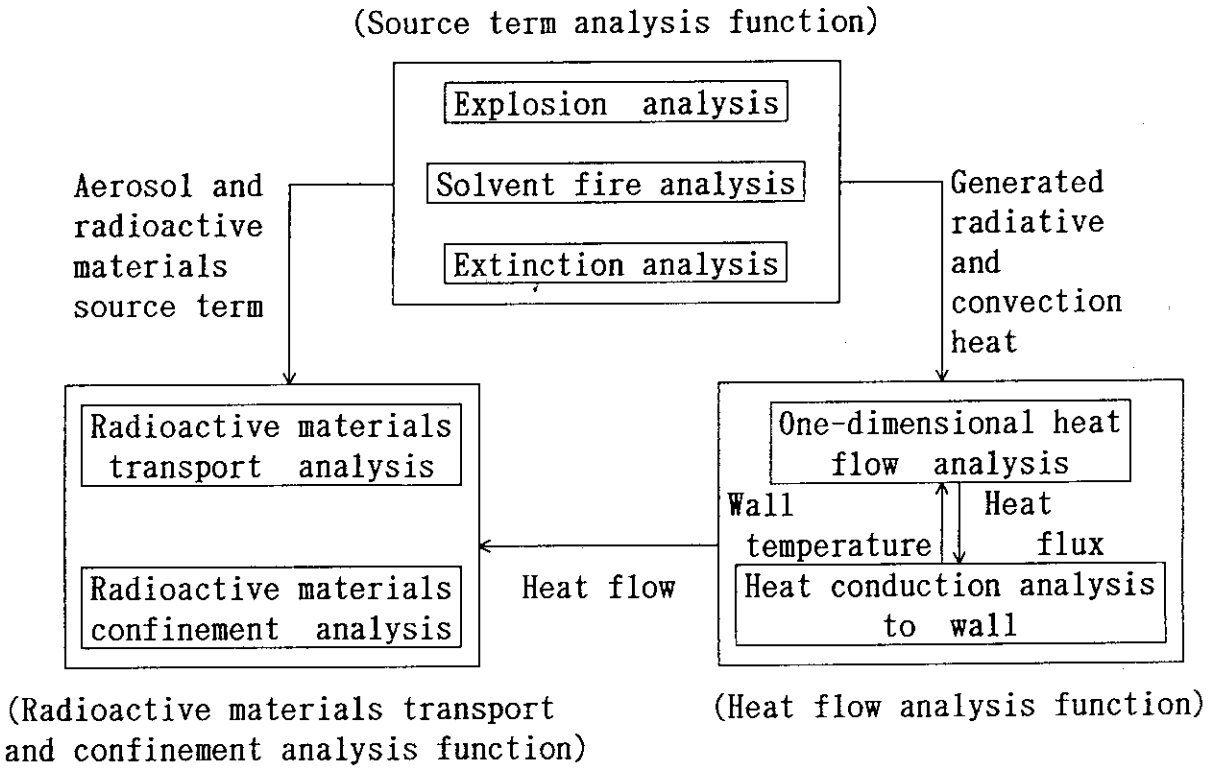

Fig. 2.2 Functions of TRANS−ACE.

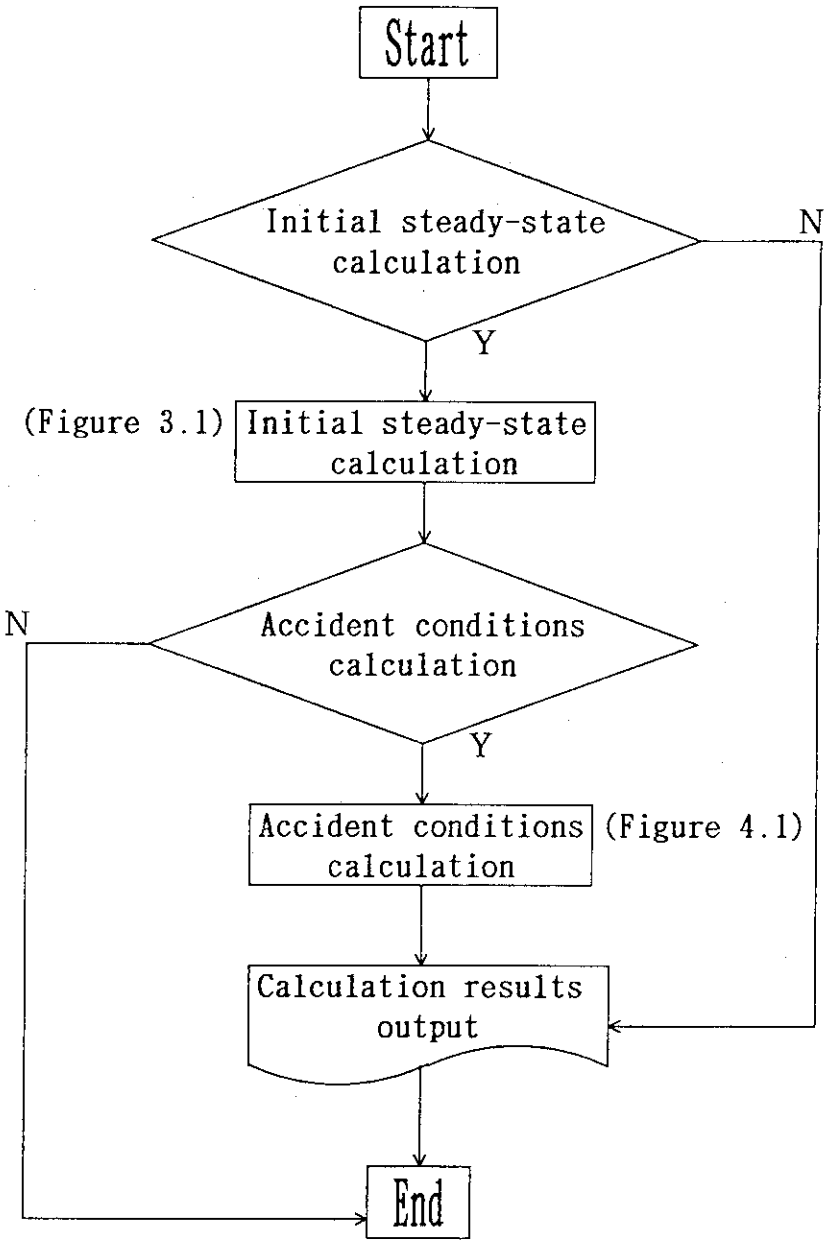

Fig. 2.3 Flow chart of TRANS-ACE.

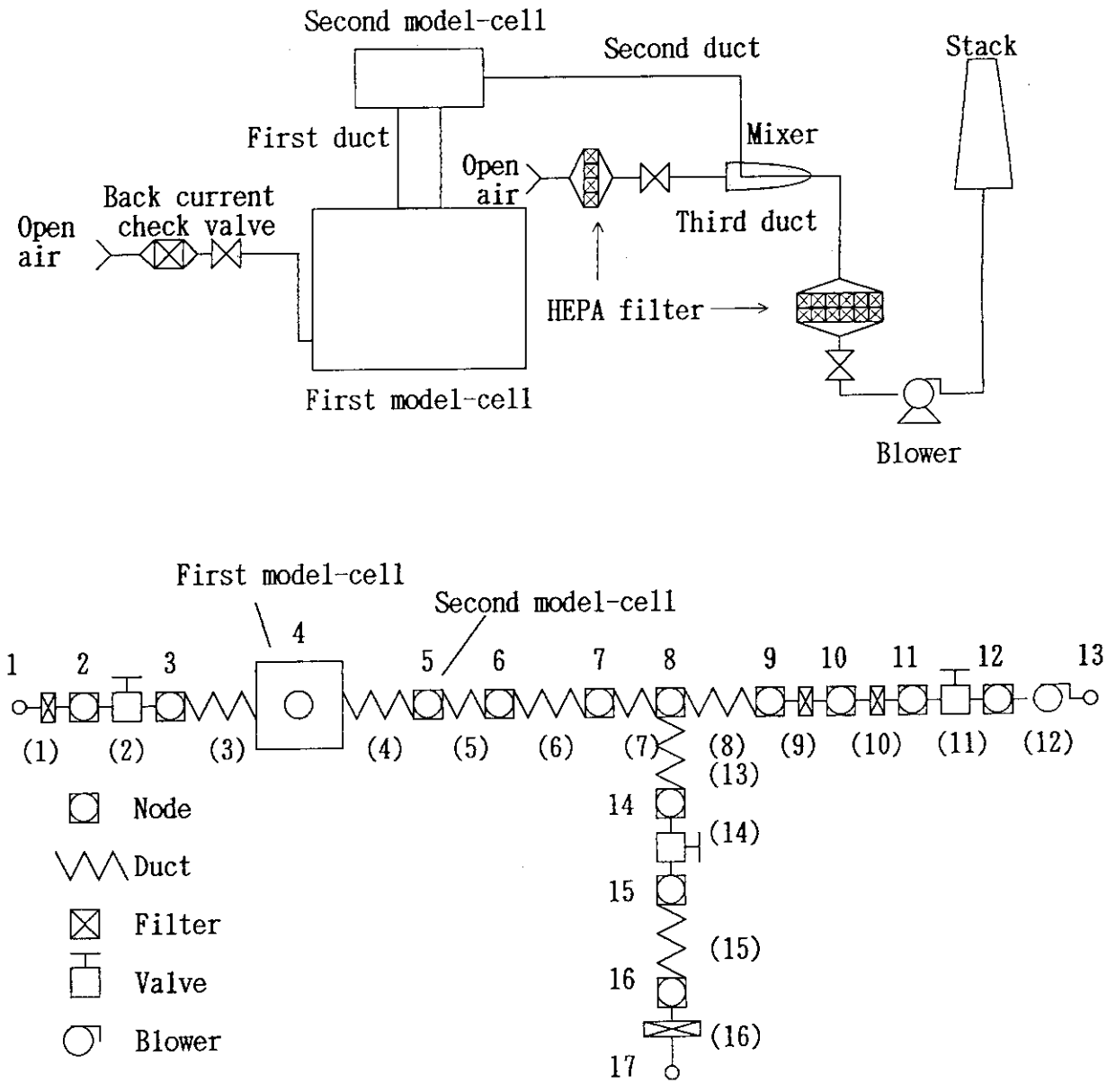

Fig. 2.4 Node junction of a sample cell-ventilation system. (Large-scale fire facility)

3. INITIAL STEADY-STATE CALCULATION IN TRANS-ACE

3.1 Outline of initial steady-state calculation

Figure 3.1 shows a flow chart of the initial steady-state calculation in the code. Initial flow resistances (ΔP) of branches are obtained from initial volume flow (Q) through branches, initial temperature (T) and pressure (P) in the nodes. Also, the resistance coefficients (K_{eff}) of branches are obtained from ΔP.

Pressure (P'), temperature (T') and density (ρ) at the nodes and volume flow (Q') at the branches are newly set by the convergence of continuous, motion, energy and state equations using initial conditions of pressure (P), temperature (T), density (ρ), volume flow (Q') and flow resistance coefficients of branches (K_{eff}) in the ventilation system. The basic equations of TRANS-ACE are the same equations as used in EVENT as follows:

(Continuous equation)

$$V \cdot \frac{d\rho}{dt} = \Sigma m_k + M_s \tag{3.1.1}$$

(State equation)

$$P = \rho \cdot R \cdot T \tag{3.1.2}$$

(Motion equation)

A.Blower: relationship between volume flow and resistance at branches is given by the user.

B.Filter:

$$\Delta P_o = \frac{K_L \cdot \mu \cdot Q}{A} + \frac{K_T \cdot \rho \cdot Q^2}{2A^2} \tag{3.1.3}$$

C.Duct and valve:

$$\Delta P = -\frac{l}{A} \cdot \frac{dm}{dt} - \frac{K_{eff}}{A^2} \cdot \frac{m \cdot |m|}{2\rho} \tag{3.1.4}$$

where, A (m^2) is the cross-sectional area of the branches, K_{eff} (-) the resistance coefficient of the branches, K_L ($m^{-1/2}$) the laminar flow resistance coefficient and K_T (-) the turbulent flow resistance coefficient, l (m) the length of branches, M_s (kg/s) the mass release rate, m (or m_k) the mass flow rate in the k-th branch, P (Pa) the pressure at nodes, ΔP (Pa) the flow resistance between two nodes, Q (m^3) the volume flow rate through branches, R (J/kg·K) the gas constant, V (m^3) the volume of node and ρ (kg/m^3) the density of fluid. Equations from (3.1.1) to (3.1.4) are programmed in TRANS-ACE from the EVENT code of the LANL. M_s is obtained by the mass release rate from solvent fire and explosion as shown in Chapter 4.2. In the initial steady-state calculation, M_s=0 is set in TRANS-ACE.

Furthermore, TRANS-ACE has a function of convergence judgment of the volume flow through the branch. The convergence is determined by the difference between flow rate Q at initial set and flow rate Q' obtained by the iteration of the above three equations. In the case of no convergence, new flow resistance was set by the movement due to openning and shutting of the relaxation valves in the ventilation system, consequently, the judgment of convergence was performed by iteration of the above three equations, as follows:

$$|Q_i - Q'_i| \leq \varepsilon \qquad (3.1.5)$$

where, i is the branch number, and ε the convergence value set by the user. The details of the movement for valves are expressed in Chapter 4.5.1.

3.2 Setting of initial flow resistances of the branches

The initial flow resistances of branches are given by the user's input or an automatic calculation. Figure 3.2 shows the flow chart of calculation of the initial flow resistances.

(1) Setting by the user's input

When the initial flow resistances are given by the user's input, the user can select one of the following two methods:

- Input of pressures in the nodes
- Input of flow resistances in the branches

In case of the former, the initial flow resistance is determined by subtracting the pressure from the upper node to lower nodes.

(2) Setting by using the automatic calculation function

When the initial flow resistances are set by the automatic calculation function, the flow resistance of each branch is calculated by Eqs.(3.2.1), (3.2.11), (3.2.15) and interpolation of Figure 3.4, as follows:

1) Automatic calculation of the flow resistance in a duct

In TRANS-ACE, it is possible to calculate the flow resistance (ΔP) for the straight duct and the elbo duct with curvature by the summation of the following equations:

$$\Delta P = \text{pressure loss due to friction of ducts} + \text{pressure loss due to reduction and magnification between cells and ducts} \tag{3.2.1}$$

A. Pressure loss due to friction of duct

$$F_k = f_c \cdot \frac{l}{D_h} \cdot \frac{\rho V_f^2}{2} \tag{3.2.2}$$

where, F_k (Pa) is the duct resistance at branch k, f_c (-) the friction factor of straight pipe, l (m) the length of duct, D_h (m) the hydraulic diameter of duct, ρ (kg/m^3) the density of fluid and V_f (m/s) the flow rate through the duct. The friction factor is given by the following equations:

(Straight duct)

$$f_c = \frac{64}{Re} \qquad (Re < 2600) \qquad (3.2.3)$$

$$f_c = 0.1\left(1.46\frac{\varepsilon_f}{D_h} + \frac{100}{Re}\right)^{0.25} \qquad (Re > 2600) \qquad (3.2.4)$$

where, Re (-) is the Reynolds number and ε_f (m) the roughness coefficient on the duct wall.

(Elbo)

$$f_c = \frac{D_h}{L}\left(0.0315\frac{R_f}{D_h} + 0.21\left(\frac{D_h}{R_f}\right)^{2.5}\right) \qquad \left(\frac{R_f}{D_h} < 1.0\right) \qquad (3.2.5)$$

$$f_c = \frac{D_h}{L}\left(0.0315\frac{R_f}{D_h} + 0.21\left(\frac{D_h}{R_f}\right)^{0.5}\right) \qquad \left(\frac{R_f}{D_h} > 1.0\right) \qquad (3.2.6)$$

where, R_f(m) is curvature of the elbo. Eq.(3.2.6) is used in the range of $0.5<(R_f/D_h)<1.0$, but in TRANS-ACE, it is used in a region even less than 0.5. If the input of hydraulic diameter of the duct is blank, D_h is given by the following equation automatically.

$$D_h = 2.0\left(\frac{A}{\pi}\right)^{0.5} \qquad (3.2.7)$$

B. Pressure loss due to a reduction and magnification between the cell and ducts

$$F_k = K_f \cdot \frac{\rho V_f^2}{2} \qquad (3.2.8)$$

where, K_f(-) is the pressure loss coefficient obtained from the following equations:

(Duct reduction)

$$K_f = 0.4(1-(\frac{A_o}{A_1})^2) \tag{3.2.9}$$

(Duct magnification)

$$K_f = (1-\frac{A_o}{A_1})^2 \tag{3.2.10}$$

where, $A(m^2)$ is the cross-sectional area of the duct (A_o/A_1).

2) Automatic calculation of the flow resistance of the valve

Flow resistances (ΔP) of butterfly valve and gate valve as shown in Fig 3.3 are calculated by the following equations:

$$\boxed{\Delta P=9800\cdot\zeta\cdot\frac{V_f'^2}{2g}} \tag{3.2.11}$$

where, ζ is the pressure loss coefficients as shown in Table 3.1, which are determined by the relation between l/d and diameter of the duct for the gate valve, and by θ for butterfly valve as input. In Eq.(3.2.11), g (m/s^2)is the gravitational constant and V_f' the flow velocity through the valve as follows:

$$V_f' = \frac{Q}{A} \tag{3.2.12}$$

where, A (m^2) is the cross-sectional area of valves in Table 3.1, which is obtained by the following equation:

(butterfly valve)

$$A=(1-\sin\theta)\cdot AMAX \tag{3.2.13}$$

(gate valve)

$$A = AMAX - \frac{1}{2}(AMAX^2\cdot\cos^{-1}(\frac{l}{d}) - \frac{AMAX(l/d)\cdot\sin(\cos^{-1}(l/d))}{\pi} \tag{3.2.14}$$

where, AMAX (m^2) is maximum cross-sectional area of the valve.

3) Automatic calculation of blower resistance

The flow resistance of blower is given by table input for the relationship between resistance (ΔP) across the blower and volume flow (Q) through the blower as shown in Figure 3.4. The interpolation among table input data is performed for blower resistance with a volume flow velocity through the blower, as follows:

A. When the volume flow was situated in the region between the two input data, resistance was given by interpolation of the straight line between two data of ΔP vs Q.

B. When the volume flow was situated at the outside of input data, resistance was given by nearest datum of ΔP vs Q in table data.

4) Automatic calculation of filter resistance

Filter resistance is calculated by using volume flow rate as follows:

$$\Delta P = \frac{K_L \mu}{A} \cdot Q + \frac{K_T \rho}{2A^2} \cdot Q^2 \qquad (3.2.11)$$

where, A (m^2) is the total area of the filter media, K_L ($m^{-1/2}$) the laminar flow resistance coefficient and K_T (-) the turbulent flow resistance coefficient for the HEPA filter as shown in Table 4.4. Q (m^3/s) is the volume flow rate through the filter. μ ($kg/m \cdot s$) is the viscosity and ρ (kg/m^3) the density of the fluid.

5) Automatic addition of check valve to prevent fluid back-flow

The flow resistance of the automatically added check valve to prevent a back-flow of the fluid at the boundary point between cell and environment is calculated by the same method of automatic calculation described for damper(see 2). If this function of automatic addition of check valve is used in the code, the flow resistance of the ventilation system must not be set by the user's input, but by the automatic calculation function described above.

(3) Adjustment of calculational error of flow resistance

Total flow resistance of the ventilation system is given by the differential pressure between inlet and outlet boundary nodes. In the automatic calculation of initial flow resistance, the total flow resistance is obtained by the summation of the flow resistances calculated for each branch in the network. However, the total flow resistance by the automatic calculation does not correspond with the differential pressure between inlet and outlet boundary nodes, because each flow resistance by automatic calculation has some amount of error. In TRANS-ACE, the error of flow resistances is compensated by adjusting open area of some valves. These error adjusting valves are set by the user's input.

The flow resistance of the valves at ΔP_e, is obtained by subtracting the flow resistance of total branches except for the valves from the differential pressure between inlet and outlet boundary nodes. The ζ-values of the valves in Eq.(3.2.11) are obtained from ΔP_e in stead of ΔP with θ (Butterfly valve) or l/d (Gate valve) in Table 3.1. Figure 3.5 shows the flow chart of the calculational error adjusting method of the valves.

Table 3.1 ζ-value of Valve

(Gate valve)

	l/d	1/8	1/4	3/8	1/2	3/4	1
ζ	1/2"	370	54	18	7.7	2.2	0.81
	1"	210	40	10	3.5	0.88	0.23
	10"	96	17	5.6	2.3	0.41	0.05

(Butterfly valve)

θ	15	10	20	30
ζ	0.24	0.52	1.54	3.91
θ	40	50	60	70
ζ	10.8	32.6	118	751

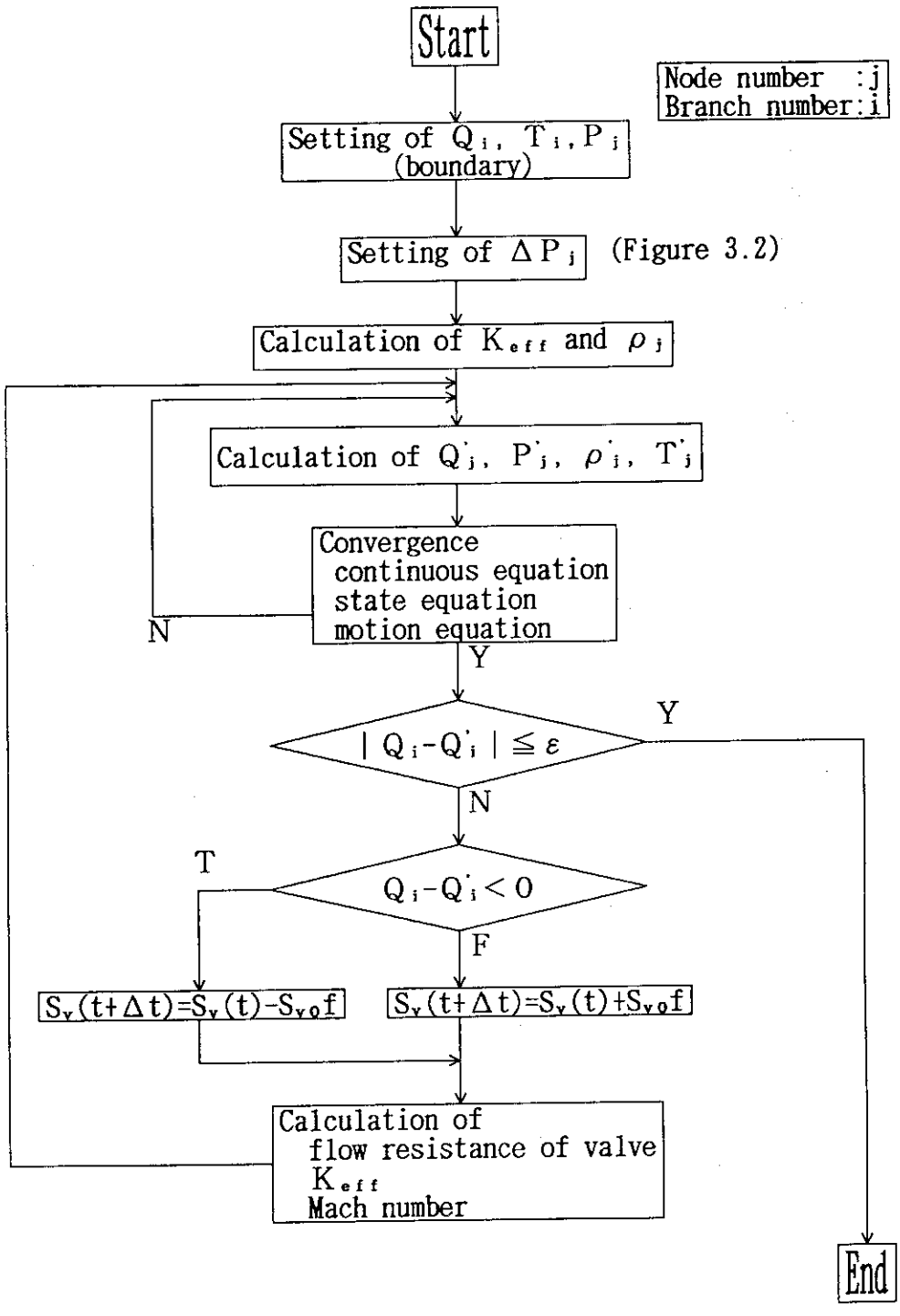

Fig. 3.1 Flow chart of the initial steady-state calculation.

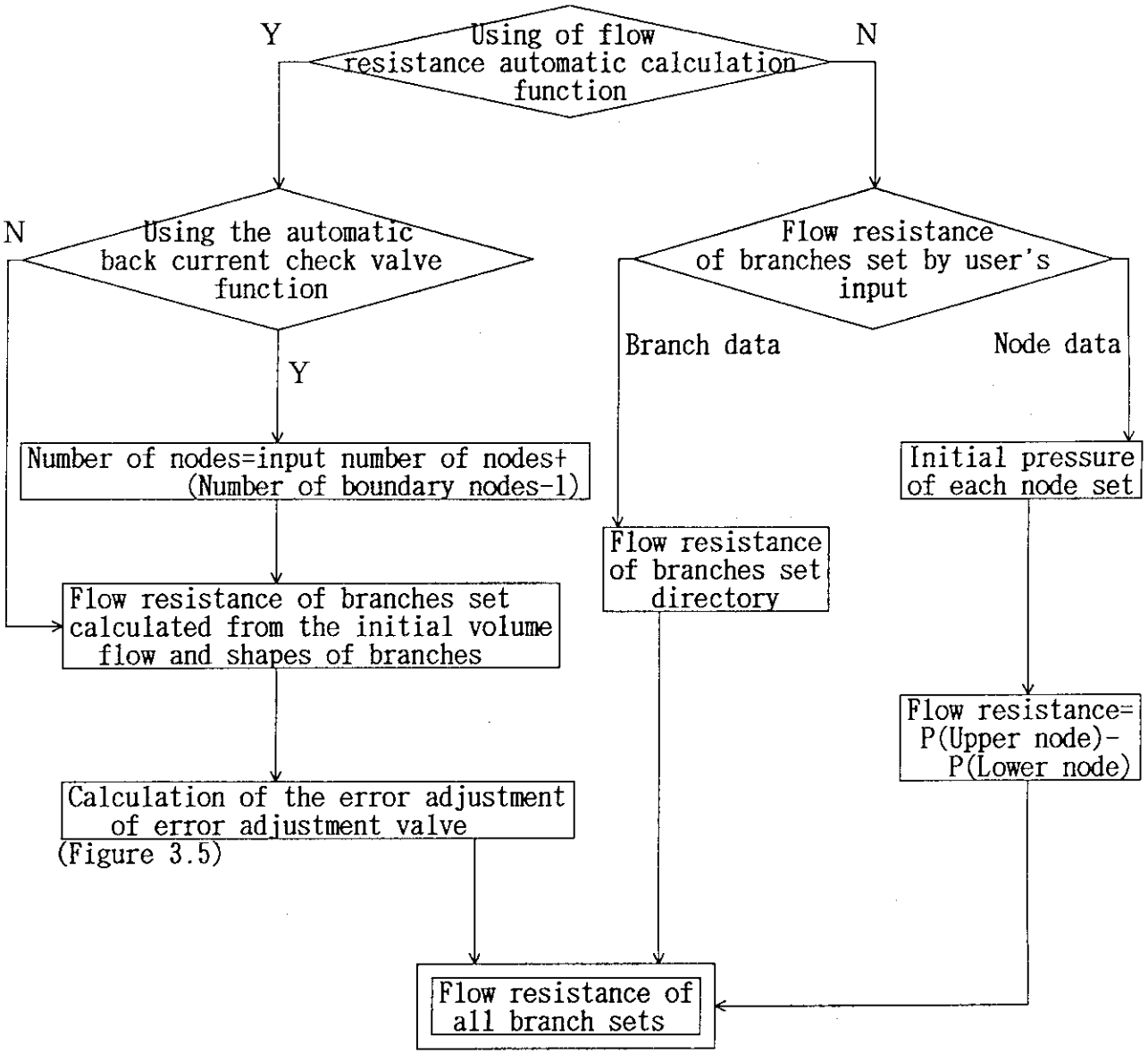

Fig. 3.2 Flow chart of the intial flow resistance calculation.

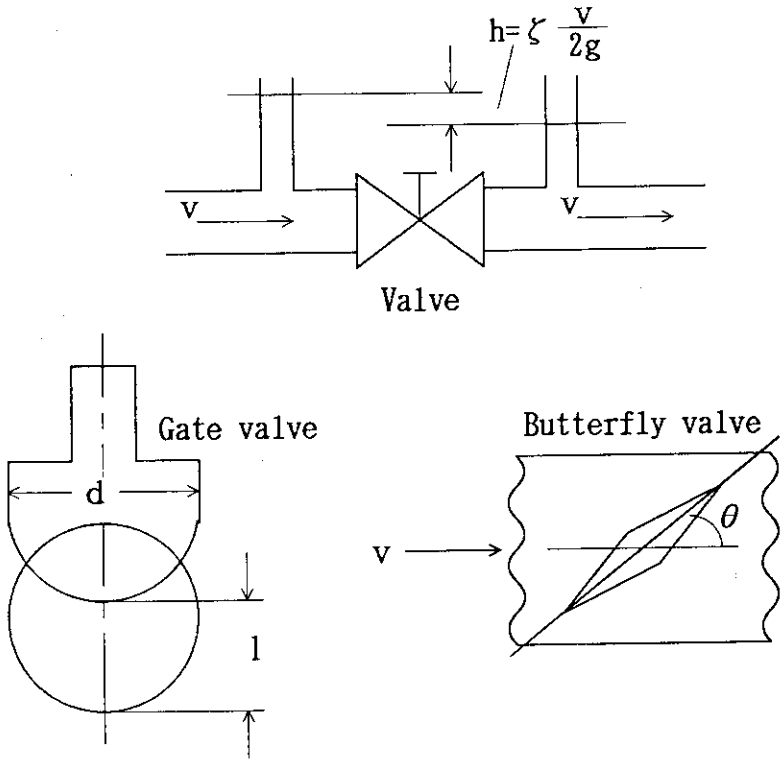

Fig. 3.3 Sketch and symbol of the valves.

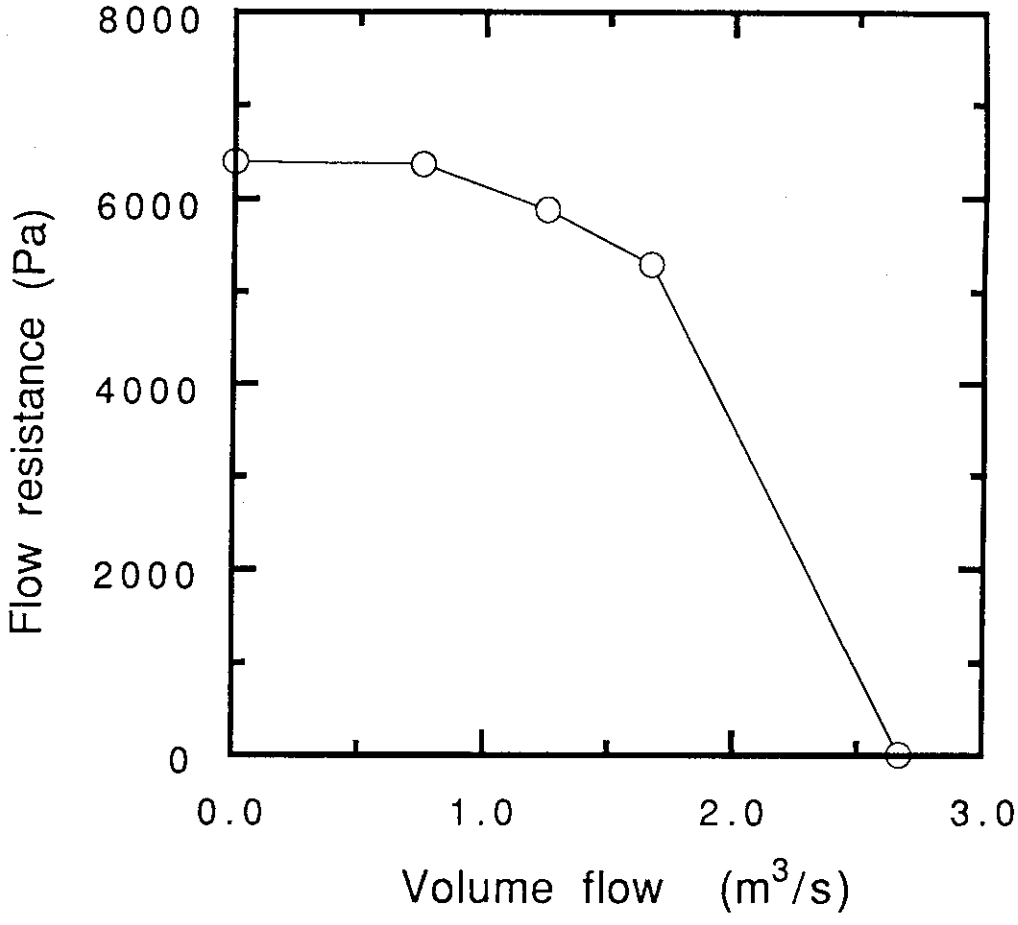

Fig. 3.4 Relationship between volume flow and flow resistance of the blower.

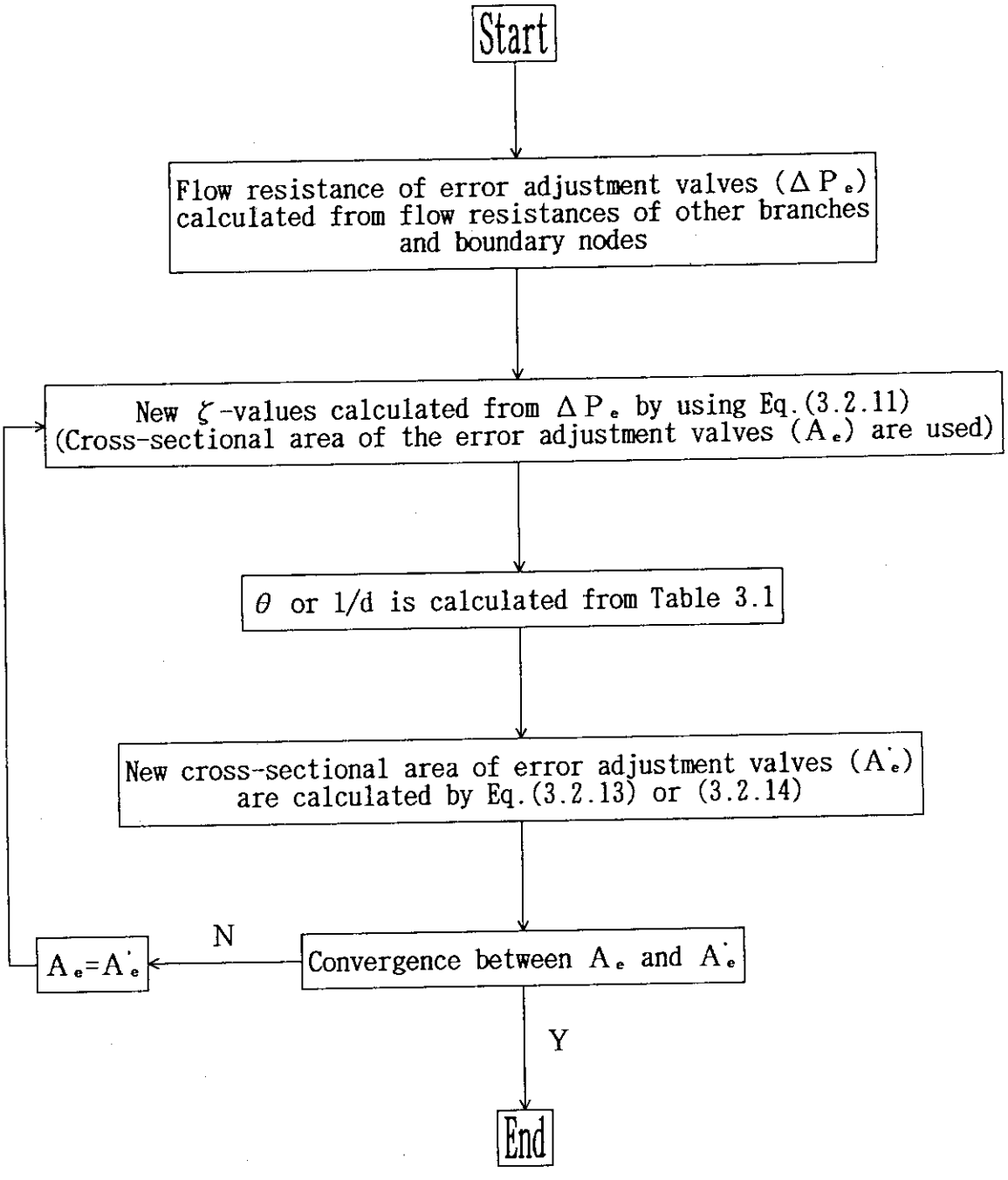

Fig. 3.5 Flow chart of error adjustment with a flow resistance automatic calculation of the ventilation system.

4. ACCIDENT CALCULATION IN TRANS-ACE

4.1 Outline of accident calculation

Figure 4.1 shows the flow chart of the calculation for thermo-fluid and airborne materials transport during fire and explosion accidents. The variation of physical values in the nodes and branches are calculated by the integration time step, $t+\delta t$.

4.2 Calculations for the source term

Analysis of source terms is necessary to calculate heat transfer and radioactive material transport in the ventilation system[6]. The accident calculations in TRANS-ACE is required to obtain source terms of the energy release rate, mass release rate and aerosol generation rate. These source terms are set in two ways: one is directory input by the user, the other by calculations of source terms in fire and explosion programmed in the code.

In the case of directory input of source terms, the user must supply one of the following combinations.

(1) Mass release rate and energy release rate of burning gas
(2) Pressure and temperature in the cell
(3) Mass release rate of burning gas and temperature in the cell

4.2.1 Analysis of a solvent fire

(1) Burning rate

Burning rate of a solvent in the cell is calculated with the pool burning model which is derived from Spalding's B-factor model in oil-droplets burning[3)4)]. The burning model was obtained from the one-dimensional burning analysis based on conservation of mass and energy of burning solvent on the pool surface in a burning pan. The burning rate of a solvent is given by

$$m_b = \xi \cdot m_{fu} = \frac{\pi \cdot d^2 \cdot h}{4(1+\delta)C_p} \ln\{(1+\delta)\cdot\varepsilon\cdot B+1\} \qquad (4.2.1)$$

$$h = \frac{\lambda \cdot Nu}{d} \qquad (4.2.2)$$

where, m_b (kg/s) is the burning rate of the solvent, d (m) the diameter of the circular burning pan, h ($J/m^2 \cdot s \cdot K$) the heat transfer coefficient of the burning pan, m_{fu} (kg/s) the consumption rate of the solvent evaporated from the pool surface in the pan. λ is the thermal conductivity ($J/m \cdot s \cdot K$). B (-) in Eq.(4.2.1) is Spalding's B-factor obtained from the following equation:

$$B = \frac{C_p(T-T_s)+f \cdot \Delta H(1-\gamma)Y_{ox}}{L_{fu} \cdot (1-\phi)} \qquad (4.2.3)$$

where, L_{fu} (J/kg) is latent heat for solvent evaporation. Burning parameters of δ, ε, ξ, f, γ, ϕ and Y_{ox} in Eq.(4.2.1) and (4.2.3) are determined from fire experiments[7] as shown in Table 4.1. These burning parameters are given by user input or calculation with empirical equations in Table 4.1.

h ($J/m^2 \cdot s \cdot K$) in the Eq.(4.2.2) is the heat transfer coefficient from fire flame to the pool surface in a pan due to natural convection expressed by the following Nusselt number:

$$Nu=3.106+0.14(Gr \cdot Pr)^{(1/3)}\{1-\exp(-0.0172 \cdot d)\} \qquad (4.2.4)$$

where Gr (-) is the Grashof number and Pr (-) is the Prandtl number.

ΔH (J/kg) in Eq.(4.2.3) is the burning heat of mixed TBP/n-dodecane solvent, this value is obtained by the following burning formulas:

(Burning of TBP)

$$(C_4H_9O)_3PO + 18O_2 \rightarrow 12CO_2 + 12H_2O + H_3PO_4$$

(Burning of n-dodecane)

$$CH_3(CH_2)_{10}CH_3 + 18.5O_2 \rightarrow 12CO_2 + 13H_2O$$

$$\Delta H = \{8100 \cdot M_C+34200(M_H-\frac{M_O}{8})-5400 \cdot M_H\} \cdot 4180 \qquad (4.2.5)$$

where, M_C, M_H and M_O are mass weight ratio of carbon, hydrogen and oxygen in the mixed solvent obtained by following equations:

$$M_C = \frac{(12\times12)(1-C_{WT})}{170.3} + \frac{(12\times12)C_{WT}}{266.3} \tag{4.2.6}$$

$$M_H = \frac{26(1-C_{WT})}{170.3} + \frac{27\times C_{WT}}{266.3} \tag{4.2.7}$$

$$M_O = \frac{(4\times16)C_{WT}}{266.3} \tag{4.2.8}$$

where, C_{WT} in the above equations is the weight fraction of TBP in the mixed solvent which is as follows:

$$C_{WT} = \frac{0.97C_{VT}}{0.97C_{VT}+0.75(1-C_{VT})} \tag{4.2.9}$$

where, C_{VT} is the volume fraction of TBP in the mixed solvent. TBP in the mixed solvent is concentrated in the burning pan during the burning of a solvent, because the boiling point of TBP is higher than that of n-dodecane. So that heat generated during the fire will be changed by the composition of mixed solvent during the fire. The change in the volume fraction of TBP (C_{VT}) in the mixed solvent is calculated with the following equation of an unit distillation of solvents:

$$\ln\frac{V_{int}}{V} = \frac{1}{\alpha_E-1}\{\ln\frac{X_{int}}{X} - \alpha_E\cdot\ln\frac{1-X_{int}}{1-X}\} \tag{4.2.10}$$

where, V_{int} and V (m^3) are the volumes of mixed solvent, X_{int} and X (-) the volume fraction of the n-dodecane at initial and during a fire. α_E (=6.33) is the ratio of relative volatility between TBP and n-dodecane. The value of ΔH in Eq.(4.2.5) can be obtained from Eqs.(4.2.6) to (4.2.10).

The energy release rate, E_s (J/s) in Eq.(4.3.1), is obtained from the following equation:

$$E_s = m_b\cdot\Delta H(1-\gamma) \tag{4.2.11}$$

where, γ (-) is the burning parameter in Table 4.1 due to the radiation of the flame of the fire.

(3) Smoke generation rate during the burning of a solvent

The particle size distribution of smoke is given as a specified distribution by the user. On the other hand, TRANS-ACE has the function to make the size distribution with input of a geometric average diameter of particles, D_g (μm), and a geometric standard deviation, σ_g (-), assuming a log-normal size distribution of smoke. The log-normal size distribution is calculated with input of D_g and σ_g for the initial size distribution with the division number (n=11 in TRANS-ACE code (see Appendix 1)).

Smoke generation rate of i-th particle, B_{Ti} (kg/s) is obtained by the following equation:

$$B_{Ti} = m_s \cdot W_{Ti} \tag{4.2.12}$$

where, m_s (kg/s) is the smoke generation rate generated by a burning solvent in the cell, W_{Ti} the weight fraction of the i-th particle in the size distribution. In JAERI's solvent fire tests, m_s is proportional to m_b as follows[8]:

$$m_s = \kappa \cdot m_b \tag{4.2.13}$$

where κ is the smoke generation coefficient which is obtained as 0.052 as dry smoke without water and solvent vapor. The smoke generation rate will be used for mass release rate of smoke, S_J, in an aerosol transport equation in Eq.(4.4.1).

(4) Gas generation rate of a burning solvent

Compositions of burning gases are assumed to be carbon dioxide, water and unburnt solvent vapor. These gas generation rates are given by the following equations:

$$B_{G,PRO} = m_b(M_{CO2}+M_{H2O})+m_{H2O} \tag{4.2.14}$$

$$B_{G,fuel} = m_{fu}-m_b = (1-\xi)m_{fu} \tag{4.2.15}$$

where, $B_{G,PRO}$ (kg/s) is the generation rate of CO_2 and H_2O, $B_{G,fuel}$ (kg/s) is the generation rate of unburnt solvent vapor. M_{CO2} (-) and M_{H2O} (-) are the weight fractions of CO_2 and H_2O. m_{H2O} (kg/s) is the evaporation rate of H_2O generated from aqueous phase through the organic solvent phase to gas phase: m_{H2O}=0 is kept to be zero before boiling of H_2O. The consumption rate of oxygen in the cell is obtained by the following equation:

$$B_{G,O2} = -m_b \cdot M_{O2} \tag{4.2.16}$$

where, M_{O2} (-) is the weight fraction of O_2 in the cell.

The mass release rate of burning gases, M_s (kg/s), is given by the following equation using equations from Eqs.(4.2.14) to (4.2.16).

$$M_s = B_{G,PRO} + B_{G,fuel} + B_{G,O2} \tag{4.2.17}$$

The value of M_s is used in continuous equation of Eq.(3.1.1) and energy equation of Eq.(4.3.1).

(5) Fire extinction

TRANS-ACE is programmed to have two fire extinction models consisting of natural extinction and boil-over burning extinction. The natural extinction model in TRANS-ACE is made with empirical equations of an extinction line between extinction and combustion regions obtained from the solvent fire tests using 30% TBP/n-dodecane and 100%n-dodecane, respectively[8]. The extinction model due to the boil-over burning is defined by a boiling time of aqueous phase under solvent phase in a pan.

The extinction line is obtained with air volume change rate of the cell, n (hr^{-1}), and the number of burning pans corresponding to the extraction process stages, s, as follows:

$$n = \frac{F}{V} \tag{4.2.18}$$

$$S = \frac{V_o}{A_o} \cdot \frac{A}{V} \tag{4.2.19}$$

where, A is burning area of the solvent pool surface in JAERI's fire tests and A_o the burning area of mixer-settlers in the extraction cell of the reference plant. F (m^3/hr) is the air ventilation flow rate. V (m^3) and V_o (m^3) are the volumes of fire test facility cell and the actual reference extraction cell of the plant. The combustion regions are calculated by following equations using the values of n and S.

100% n-dodecane fire : $n - 0.309 \cdot S^{1.6}$ (4.2.20)

30% TBP/n-dodecane fire : $n - 2.01 \cdot S^{1.2}$ (4.2.21)

If the fire condition is located outside of the combustion region, natural extinction occurs due to a lack of oxygen in the cell[9]. In this case, the limited burning concentration of oxygen in the cell is C_e=0.127 mol%[8]. The time of natural extinction, t_e (s), is obtained from the material balance of oxygen in the fire cell by using m_b (kg/s) and F (m^3/hr), as follows:

$$t_e = -\frac{V}{F}\cdot\ln\{1-\frac{F(C_o-C_e)}{3.48\cdot m_b}\} \qquad (4.2.22)$$

where, C_o (kg/m^3) is the oxygen concentration in air at the inlet of the cell.

On the other hand, the boil-over burning extinction is initiated by water boiling under the solvent phase due to the rise of the water temperature in the burning pan. During the-boiling of water, a large amount of solvent vapor is vaporized into the cell atmosphere by steam distillation due to steam bubbles passing through the solvent phase in the pan. The boil-over burning occurs in the cell atmosphere by an explosion of solvent vapor in the fire cell. After boil-over burning, the extinction occurs due to a lack of oxygen caused by the explosion. The extinction time of solvent fire, t_e (s), is obtained by the following equation:

$$t_e = \frac{L_{org}}{V_s} - \frac{\lambda}{C_p\cdot\rho_{org}\cdot V_s}\ln\frac{T_b-T_o}{T_L-T_o} \qquad (4.2.23)$$

where, L_{org} (m) is the initial height of the solvent phase in the burning pan, V_s (m/s) the decreasing rate of the solvent layer in the pan, T_b (°C) the boiling temperature of n-dodecane (=216.3), T_L (°C) is the boiling temperature of water (=100) and T_o (°C) the temperature of the aqueous phase near the bottom of the pan. V_s is obtained using the following equation:

$$V_s = V_c+V_T\{1-\exp(-0.0172d)\} \qquad (4.2.24)$$

where, d (m) is the diameter of the burning pan, V_c (m/s) the decreasing rate of the solvent layer caused by heat conduction through the free board of pan wall except for natural convection, V_T (m/s) the decreasing rate of the solvent layer due to the

turbulent heat transfer from a fire flame to the solvent pool surface. Both decreasing rates of the solvent layer where obtained as follows:

$$V_C = 3.106 \frac{\mu}{(1+\delta)\cdot\sigma_{fu}} \ln\{(1+\delta)\cdot\varepsilon\cdot B+1\}\cdot Pr^{-1}\cdot\frac{1}{d} \qquad (4.2.25)$$

$$V_T = 0.14 \frac{\mu}{(1+\delta)\cdot\sigma_{fu}} \ln\{(1+\delta)\cdot\varepsilon\cdot B+1\}\cdot Pr^{(-2/3)}\{\frac{g\cdot\beta\cdot\Delta T\cdot P^2\cdot M^2}{R^2\cdot T_S^2\cdot\mu^2}\} \qquad (4.2.26)$$

where, μ (Pa·s) is the gas viscosity, σ_{fu} (kg/m^3) the density of solvent, g (m/s^2) the gravitational acceleration constant and β (K^{-1}) the volume expansion constant. T_s (K) is the temperature at the solvent surface, ΔT (K) the temperature difference between the fire flame and solvent pool surface, P (atm) the pressure in the cell, M is the molecular weight of the fluid and R (J/kg·K) the gas constant. δ (-) and ε (-) are the burning parameters which can be seen in Table 4.1. B (-) is the Spalding's B-factor in Eq.(4.2.3).

4.2.2 Analysis of explosion

The explosion model in TRANS-ACE is the same model as in the EVENT84[5]. In this explosion model, energy release rate E_s (J/s) and mass release rate M_s (kg/s) are calculated from total explosion energy E_T (J) and total amount of mass release M_T (kg) of explosive materials and decayed time of explosive pressure wave in a cell.

(1) Calculation of total energy

TRANS-ACE is programmed, similar to the program in EVENT84, for TNT(tri-nitro-toluene), hydrogen, acetylene and red-oil formed by nitro-reaction of TBP.

The chemical reactions with the explosion of hydrogen and acetylene are as follows:

(Explosion of hydrogen)

n<2m

$$nH_2 + mO_2 \rightarrow nH_2O + (m-0.5n)O_2 \qquad (4.2.27)$$

n>2m

$$nH_2 + mO_2 \rightarrow 2mH_2O + (n-2m)H_2 \qquad (4.2.28)$$

(Explosion of acetylene)

$n<0.4m$

$$nC_2H_2 + mO_2 \rightarrow 2nCO_2 + (2m-5n)O_2 + nH_2O \quad (4.2.29)$$

$n>0.4m$

$$nC_2H_2 + mO_2 \rightarrow 0.8mCO_2 + 0.4nH_2O + (n-0.4m)C_2 \quad (4.2.30)$$

The internal energy of the i-th burning gas is given by the following equation:

$$u_i = \int_0^T C_{vi} \cdot dT \quad (4.2.31)$$

where, u_i (J/mol) is the internal energy of the i-th burning gas, C_v (J/mol·K) the heat capacity of the constant volume. Consequently, total explosion energy E_T (J) generated by the burning gases is obtained as follows:

$$E_T = \sum_{i=1}^{N} (n_{o,i}, u_i) \quad (4.2.32)$$

where, $n_{o,i}$ (mol) is mole number of the i-th burning gas due to the explosion.

On the other hand, total explosion energy E_T (J) of red-oil is calculated with the heat generation of TNT by converting the red-oil mass into an equivalent mass of TNT.

$$E_T = 1944 \cdot F_c \cdot M_T \cdot F_{eq} \quad (4.2.33)$$

where, 1944 (J/kg) is the heat generation of TNT, F_c (-) the heat generation coefficient depends on the size of cell (=2.5), F_{eq} (-) the conversion coefficient of the mass to TNT. F_{eq}=1.0 is adopted for TNT and F_{eq}=1.32 for red-oil.

(2) Calculation of the energy release rate and mass release rate

The decayed time of explosive pressure wave for burning the weight of M_T (kg) is determined by the following equation taking into consideration the equilibrium by reflection and attenuation of pressure wave in the cell:

$$t = F_a\left(\frac{L}{C_{sv}}\right) \quad (4.2.34)$$

where, F_a (-) is a constant value from 4 to 8 depending on the kind of explosive materials, L (m) the representative length of the cell, C_{sv} (m/s) the speed of sound. A simple triangular spike such as in Figure 4.2 is made by using the total explosion energy, E_T, or the total amount of mass release, M_T, and this decayed time. The area of a simple triangular spike becomes the total amount of mass release and total energy release, so that maximum mass release rate M_{sm} (kg/s) and maximum energy release rate E_{sm} (J/s) in the triangle can be obtained by following equations:

$$M_{sm} = M_T \left(\frac{2}{t}\right) \tag{4.2.35}$$

$$E_{sm} = E_T \left(\frac{2}{t}\right) \tag{4.2.36}$$

The triangular spike shows the time function of the energy release rate, E_s, or the mass release rate, M_s. These mass and energy release rates correspond to the mass and energy release rates in Eqs.(3.1.1) and (4.3.1), respectively.

4.2.3 Release of radioactive materials

(1)Inventory of radioactive materials

TRANS-ACE can calculate inventory of radioactive materials before an accident occurs by

1) user input for each nuclide,
2) table input of radioactive materials at cooling time of 4 years for 45 GWD/tU burn-up in a nuclear fuel reprocessing plant as shown in Table 4.2, and
3) table input of radioactive materials in a small-scale reprocessing plant at the cooling time of 180 days for 28 GWD/tU burn-up as shown in Table 4.3.

The inventory of radioactive materials above is obtained by ORIGEN2[10] for 4.5% initially enriched uranium fuel.

(2) Release of radioactive aerosol in a fire

Amounts of radioactive materials in the extraction process are distributed between the solvent and aqueous phases by their corresponding distribution coefficients, D (-). Tables 4.2 and

4.3 show concentrations of radioactive materials at the equilibrium state and their distribution coefficients[11].

In boil-over burning during a solvent fire, the distribution coefficient increases rapidly due to the hot-water droplets in the solvent dispersed by the water boiling during the solvent phase, and the TBP in the solvent will be concentrated in the burning pan. The increase in the distribution coefficients is evaluated by the following empirical equation obtained by JAERI's fire tests[6]:

$$D_B = 4.66 \cdot D_{int}^{0.855} \tag{4.2.37}$$

where, D_B is the distribution coefficient after the boil-over burning and D_{int} the initial distribution coefficient before boil-over burning, respectively.

The release rate of the i-th radioactive nuclide, $m_{F,i}$ (Ci/s), from the burning pan to the gas phase is proportional to entrainment of the i-th nuclide and solvent consumption rate during a fire, as follows:

$$m_{F,i} = e_{F,i} \cdot m_{fu} \frac{D_i \cdot C_{w,i}}{\rho_{org}} \tag{4.2.38}$$

where, m_{fu} (kg/s) is the consumption rate of the solvent from the pan during a fire, D_i the distribution coefficient of the i-th nuclide, $C_{w,i}$ the concentration of the i-th nuclide in the aqueous phase under the solvent and ρ_{org} (kg/l) the density of the solvent. $e_{F,i}$ (-) is the entrainment coefficient of the i-th nuclide during a fire determined by the following equation:

$$e_{F,i} = \frac{\text{(transport rate of radioactive nuclides to gas phase)}}{\text{(transport rate of all radioactive nuclides to gas phase with solvent vapor)}} \tag{4.2.39}$$

Values of e_F are obtained experimentally as from 0.05 to 0.4 for Cs, from 0.0005 to 0.005 for Sr, from 0.01 to 0.3 for Ru, less than 0.01 for Ce and from 0.00003 to 0.0008 for U by JAERI's fire tests[6]. In boil-over burning, the entrainment coefficients become large due to the direct transport of the nuclides with water vapor from the aqueous phase through into the gas phase. In the TRANS-ACE, $e_{F,i}$=1 is given for each nuclide during boil-

over burning.

Radioactive nuclides released become aerosol in the fire flame, except for the volatile nuclides. The aerosol adheres to smoke particles due to the coagulation in the flame. In TRANS-ACE, the release rate ratio of the airborne nuclides to smoke, ω (Ci/kg), is defined by

$$\omega = \frac{m_F}{\dot{m}_s} = \frac{e_F \cdot D \cdot C_w}{\chi \cdot \xi \cdot \rho_{org}} \tag{4.2.40}$$

where, m_F (Ci/s) is the release rate of airborne radioactivity as expressed by Eq.(4.2.38), m_s (kg/s) is the generation rate of smoke by Eq.(4.2.13). The airborne concentration of the i-th radioactive i-th nuclide, $C_{Fi,j}$ (Ci/m^3), is obtained from the value of ω_i and the concentration of smoke $C_{s,j}$ at the node-j in the ventilation system.

$$C_{Fi,j} = \omega_i \cdot C_{s,j} \tag{4.2.41}$$

(3) Release of radioactive aerosol by the explosion

It is assumed that smoke aerosol of M_{sp} (kg) and liquid droplets of M_{H2O} (kg) containing radioactive materials will generate in the cell by the explosion. The radioactive aerosol of M_a (kg) is formed due to the evaporation of the liquid droplets by the explosion heat. If the weight of the airborne aerosol in the cell is M_p (kg), the following equation is given as:

$$M_p = M_{sp} + M_a \tag{4.2.42}$$

Since solute containing radioactive materials existed in the liquid droplets, M_p is:

$$M_p = M_{sp} + \frac{C_o \cdot M_{H2O}}{\rho_{H2O}} \tag{4.2.43}$$

where, M_{H2O} is the weight of the liquid droplet, C_o (kg/m^3) the concentration of solute in the liquid droplet and ρ_{H2O} (kg/m^3) the density of the liquid droplets. In TRANS-ACE, as many as 20 radioactive nuclides are given as table input and their radioactivity, Γ_i (Ci/l), obtained by ORIGEN2.

The release rate ratio of the i-th nuclide as aerosol, ω_i (Ci/kg), is obtained from Eq.(3.1.45):

$$\omega_i = \frac{M_{F,i}}{M_P} \tag{4.2.44}$$

where, $M_{F,i}$ (Ci) is the radioactivity of the i-th nuclide released in the cell at the explosion, using the value of Γ, as follows:

$$M_{F,i} = \frac{M_a \cdot \Gamma_i}{C_o} \tag{4.2.45}$$

Accordingly, ω_i can be calculated from the following equation:

$$\omega_i = \frac{M_a \cdot \Gamma_i}{C_o (M_{sp} + M_a)} \tag{4.2.46}$$

The concentration of the i-th radioactive nuclide in the j-th cell, $C_{Fi,j}$ (Ci/m³), is obtained with ω_i and the smoke concentration, $C_{s,i}$, as follows:

$$C_{Fi,j} = \omega_i \cdot C_{sj} \tag{4.2.47}$$

4.2.4 Generation and transportation of radioactive gases

Volatile nuclides such as tritium, iodine and ruthenium tetraoxide are released from the source in the cell and transported through the duct of the ventilation system. The calculation of transport of gases containing radioactive gases is important, because they can not be trapped by the filter in the ventilation system. In TRANS-ACE, the fractional gasification of radioactive volatile materials, η, are given in the input data. The concentration of gases containing radioactive volatile materials in the j-th node, C^*_j (kg/m³), is calculated by the following equation:

$$V_j \frac{dC_j^*}{dt} = \sum_k^N C_k^* \cdot v_k \cdot A_k + \eta \cdot m_F \tag{4.2.48}$$

where, V_j (m³) is the cell volume of the jth-node, v_k (m/s) the flow rate through k-th branch, A_k (m²) the cross-sectional area of k-th branch and Σ the summation of all branches connected at the j-th node.

4.3 Heat and fluid flow calculations

4.3.1 Heat transfer analysis in cells and ducts

(1) Heat transfer equations for cells and ducts

In TRANS-ACE, compressibility and temperature of the fluid are obtained at the nodes, and the mass and volume flow rate are obtained at the branches from an upper node and lower node in the same way as in EVENT.

Basic equations of the heat transfer analysis are continuous equation (Eq.(3.1.1)), state equation (Eq.(3.1.2)) and energy equation for the nodes and motion equation (Eq.(3.1.3) or Eq.(3.1.4)) for the branches.

(Energy equation)

$$\frac{dP}{dt} = \frac{R}{C_v V}[\Sigma\{m_k(C_p T_k + \frac{V_k^2}{2}) - q_D\} + M_s C_p T_s + E_s - q_c] \qquad (4.3.1)$$

where, C_p (J/kg·K) and C_v (J/Kg·K) are the heat capacities of constant pressure and constant volume, E_s (J/s) the energy release rate, M_s (kg/s) the mass release rate, m_k (kg/s) mass flow rate at the k-th branch, P (Pa) pressure at the node, R (J/kg·K) the gas constant, T_k (K) the temperature at the inlet of the k-th branch, T_s (K) the temperature of the mass release source and v_k (m/s) the flow rate at the k-th branch.

Heat transfer of q_D and q_C in Eq.(4.3.1) are obtained by the following equations.

$$q_D = \alpha_{in}(T_g - T_{w1}) \qquad (4.3.2)$$

$$q_C = \alpha_{in}(T_g - T_{w1}) + J_{rad} \qquad (4.3.3)$$

where, q_D (J/s) is the heat transfer toward the duct walls and q_C (J/s) the heat transfer toward the cell walls. J_{rad} (J/s) is the heat flow toward the cell wall due to radiation, T_g (K) the gas phase temperature, T_{w1} (K) the temperature of duct and cell walls and α_{in} (J/s·m²·K) the heat transfer coefficient.

Energy release rate, E_s (J/s), and mass release rate, M_s (kg/s), were already shown in Chap. 4.2 for a solvent fire and explosion.

(2) Connection between the node and branch

The variation of the state values at the connection between a node and branch is obtained by assuming the adiabatic change in pressure, temperature and density at a node at the upper position of the branch, as follows:

$$\frac{P_j}{P_i} = \left(\frac{T_j}{T_i}\right)^{\gamma_c/(\gamma_c-1)} \tag{4.3.4}$$

$$\frac{\rho_j}{\rho_i} = \left(\frac{T_j}{T_i}\right)^{1/(\gamma_c-1)} \tag{4.3.5}$$

$$\rho_i \cdot V_i \cdot A_i = \rho_j \cdot V_j \cdot A_j \tag{4.3.6}$$

$$T_i + \frac{V_i^2}{2C_p} = T_j + \frac{V_j^2}{2C_p} \tag{4.3.7}$$

where, subscripts i and j mean the positions at the i-th node and j-th branch and γ_c the heat capacity ratio ($=C_p/C_v=1.4$). By using Eqs.(4.3.4) to (4.3.7), the following equations are obtained as:

$$T_i + \frac{Q_i^2}{2C_p \cdot A_i^2}\left(\frac{T_j}{T_i}\right)^5 = T_j + \frac{Q_j^2}{2C_p \cdot A_j^2} \tag{4.3.8}$$

$$\rho_j = \left(\frac{T_j}{T_i}\right)^{2.5} \tag{4.3.9}$$

The pressure at the entrance of the j-th branch is also obtained by the following equation:

$$P_j = \rho_j \cdot R \cdot T_j \tag{4.3.10}$$

If a node before a branch is the boundary node at the inlet or outlet of the ventilation system, the cross-sectional area of the boundary node is obtained by the following equation:

$$A_i = \frac{A_j}{0.01 \cdot \mathrm{CONVERGE}} \tag{4.3.11}$$

where, CONVERGE is a convergence value judgment.

(3) Choking model

TRANS-ACE is programmed to use the choking model in the case of large-scale flow rate conditions. If the critical mass flow, m_{CR} (kg/s), is larger than m (kg/s) given by the motion equation of Eq.(3.1.1), m_{CR} is used as obtained by the following equation instead of m as:

$$m_{CR} = \rho_J \cdot V_J \cdot A = A \cdot M_J \cdot (\gamma_J \cdot P_J \cdot \rho_J)^{0.5} \tag{4.3.12}$$

where, M_J (-) is a Mach number obtained by the following equation:

$$K_{eff} = \frac{1-M_J^2}{\gamma_c \cdot M_J^2} + \frac{\gamma_c+1}{2\gamma_c} \ln\{\frac{(\gamma_c+1)M_J^2)}{2+(\gamma_c-1)M_J^2}\} \tag{4.3.13}$$

where, K_{eff} is the resistance coefficient expressed by Eq.(3.1.4).

(4) Calculational method

Basic equations from Eqs.(3.1.1) to (3.1.4) and (4.3.1) are calculated by the complete implicit solution method. They are obtained by the Newton's method by iteration calculations of pressure and density. The boundary conditions of basic equations are assumed by the constant value of pressure, temperature at the nodes containing boundaries in the ventilation system.

4.3.2 Heat conduction analysis in cells and ducts

(1) Basic equations of heat conduction

Basic equations of heat conduction are obtained as:

$$\rho_w \cdot C_{p,w} \cdot \frac{\partial T}{\partial t} = \lambda \cdot \frac{\partial^2 T}{\partial x^2} \tag{4.3.14}$$

$$-\lambda \cdot \frac{\partial T}{\partial x}\bigg|_{x=0} = \alpha_{in}(T_g - T_{w1}) + J_{rad} \tag{4.3.15}$$

$$-\lambda \cdot \frac{\partial T}{\partial x}\bigg|_{x=d} = \alpha_{out}(T_{wo} - T_o) \tag{4.3.16}$$

where, $C_{p,w}$ (J/kg·K) is the specific heat of the wall in the cells and ducts, J_{rad} (J/m²·s) the heat flux of the radiative flow (J=0 at duct), T (K) the temperature on the walls, T_g (K)

the temperature of the gas, T_o (K) the temperature of the atmosphere, T_{wi} (K) the temperature on the inner surface of a wall and T_{wo} (K) the temperature on the outer surface of a wall. x (m) is the thickness of a wall (x=0:inside wall, x=d:outside of a wall). α_{in} (J/m²·s·K) is the heat transfer coefficient from gas to the inner surface of a wall, α_{out} (J/m²·s·K) the heat transfer coefficient from the outer surface of a wall. λ (J/m·s·K) is the thermal conductivity of the wall materials and ρ_w (kg/m³) the density of a wall.

(2) Radiative heat flow from gas to wall in a cell

1) Cell containing accidents

The heat fluxes of radiative flow to the wall in a cell during a fire or explosion, J_{rad} (J/m²·s), are calculated by the following equation:

(Fire accident)

$$J_{rad} = \varepsilon_o \cdot \sigma \cdot (T_g^4 - T_{wi}^4) + \frac{\Delta H \cdot m_b \cdot \gamma}{A_{wi}} \qquad (4.3.17)$$

(Explosion accident)

$$J_{rad} = \varepsilon_o \cdot \sigma \cdot (T_g^4 - T_{wi}^4) + \frac{E_{ST} \cdot \gamma_{ST}}{A_{wi}} \qquad (4.3.18)$$

where, σ (-) is the radiation coefficient, ε_o (J/m²·s·K⁴) the Stefan-Boltzmann constant, ΔH (J/kg) the heat generation of a burning solvent. A_{wi} (m²) is the total surface area of the inner wall in a cell, m_b (kg/s) the burning rate of a solvent, $\Delta H * m_b$ the heat generation rate by a fire, E_{ST} (J/s) the heat generation rate by an explosion and γ_{st} (-) the total radiative effects by the explosion.

2) Cells outside of an accident

The heat flux of the radiative heat flow, J_{rad} (J/m²·s), is obtained as follows:

$$J_{rad} = \varepsilon \cdot \sigma (T_g^4 - T_{wi}^4) \qquad (4.3.19)$$

(3) Convective heat transfer coefficient for cells and ducts

The calculation of heat transfer coefficient in a turbulent flow is obtained by the heat transfer coefficient, α_{in} ($J/m^2 \cdot s \cdot K$) involving the Nusselt number, in a smooth flat plane or pipe as follows:

$$\alpha_{in} = \lambda \cdot Nu/D_a \tag{4.3.20}$$

where, Nusselt number, Nu, is calculated from:

$$Nu = 0.023 \cdot Re^{0.8} \cdot Pr^{0.4} \quad \text{(duct)} \tag{4.3.21}$$

$$Nu = 0.037 \cdot Re^{0.8} \cdot Pr^{(1/3)} \quad \text{(cell)} \tag{4.3.22}$$

where, D_a (m) is the representative height of a cell or diameter of the duct. Pr(-) is the Prandtl number, Re (-) the Reynolds number, respectively. λ ($J/m \cdot s \cdot K$) is the heat conductivity of gas.

(4) Heat transfer coefficient from the outer wall to the atmosphere

The natural convection heat transfer from the outer wall to the atmosphere is obtained by the equation for vertical face in a cell and duct, neglecting curvature. The diameter of an inclined duct is obtained by $D_a/\cos\phi_d$ instead of the representative diameter (D_a).

The heat transfer coefficient from the outer wall to the atmosphere, α_{out} ($J/m^2 \cdot s \cdot K$), is obtained by the following equation:

$$\alpha_{out} = \lambda \cdot Nu/D_a \tag{4.3.23}$$

where, Nu is obtained by

$$Nu = 0.1(Gr \cdot Pr)^{(1/3)} \quad \text{(cell, } \phi_d > 80^\circ \text{ of duct)} \tag{4.3.24}$$

$$Nu = 0.53(Gr \cdot Pr)^{(1/4)} \quad (\phi_d < 80^\circ \text{ of duct)} \tag{4.3.25}$$

where, Gr (-) is the Grashof number, Pr (-) the Prandtl number.

4.4 Confinement of radioactive materials

4.4.1 Transport equation of an aerosol

The basic equation of aerosol transport is given by Eq.(4.4.1) at the j-th node.

$$V_j \frac{dC_j}{dt} = C_j \sum_{k=lb} v_k \cdot A_k + \sum_{k=ub} C_k v_k (1-E_{to,k}) A_k + S_{g,j} - S_{d,j} \qquad (4.4.1)$$

where, subscripts lb and ub mean the lower and upper branches of the j-th node, respectively. C_j (kg/m^3) is the concentration of an aerosol at the j-th node, C_{un} (kg/m^3) the concentration of aerosol at the upper node of the j-th node. A_k (m^2) is the cross-sectional area of the k-th branch, v_k (m/s) the flow rate at the k-th branch and $E_{to,k}$ (-) the deposition efficiency of an aerosol at the k-th branch. $S_{g,j}$ (kg/s) is the source term of aerosol at the j-th node as shown in Chap. 4.2.1(3), $S_{d,j}$ (kg/s) the deposition rate of aerosol at the j-th node. V_j (m^3) is the volume of the j-th node and Σ the summation for branches connected with at the j-th node.

4.4.2 Aerosol deposition

The aerosol deposition model is considered in TRANS-ACE for the diffusional, gravitational and thermophoretic depositions, respectively.

(1) Deposition of aerosol in the duct

1) Deposition efficiency of an aerosol

The aerosol deposition efficiency in Eq.(4.4.1), E_{to}, is determined by Eq.(4.4.2) and its deposition rate on the wall, v_a (m/s), is also by using Eq.(4.4.3).

$$E_{to} = \frac{C_o - C_1}{C_o} \qquad (4.4.2)$$

$$v_a = \frac{v_{ave} \cdot R_d}{2L} \ln(1-E_{to}) \qquad (4.4.3)$$

where, C_o and C_1 (kg/m^3) are the concentrations of aerosol in upper and lower cells. L (m) is the length of the branch, R_d (m) the radius of the duct. v_a (m/s) is the aerosol deposition rate and v_{ave} (m/s) the flow rate of fluid through a duct. Consequently, $S_{d,j}$ in Eq.(4.4.1) is obtained by the following equation:

$$S_{d,j} = S \cdot v_{a,j} \cdot C_j \qquad (4.4.4)$$

where, S is the surface area of the deposition.

2) Aerosol deposition due to diffusional and gravitational mechanisms

Kanaoka's aerosol deposition model[12] is used in TRANS-ACE for diffusional and gravitational depositions of aerosol in a duct. Here the deposition efficiency of aerosol in a cell, E_{to}, is obtained by Eq.(4.4.5) and the aerosol deposition rate in Eq.(4.4.3) is also calculated from E_{to}.

$$E_{to} = 1-\exp(-2\frac{S_{tav}}{v_{av}^{+}}\frac{L}{R}) \tag{4.4.5}$$

$$S_{tav} = \frac{1}{\pi}\int_{0}^{\pi} S_t^{+} d\theta \tag{4.4.6}$$

where, S^{+} (-) is Stokes number with S^{+} (-), the dimensionless stopping parameter of an aerosol particle toward the wall, as indicated by the following equations:

$$S^{+} = \frac{0.9\cdot\rho_p\cdot D_p\cdot u^{*2}}{18\cdot\mu\cdot\nu} \tag{4.4.7}$$

$(S^{+}\leqq 5)$

$$\frac{1}{S_t^{+}} = \frac{u^{*}}{u_t\cdot\cos\theta}[1-\exp\{\frac{14.5^3}{2}\frac{u_t}{u^{*}}\cos(\frac{1}{25}-\frac{1}{S^{+}})\}]+10.75+v_{av}^{+}+F(30) \quad (\theta\neq\frac{\pi}{2}) \tag{4.4.8}$$

$$\frac{1}{S_t^{+}} = \frac{14.5^3}{2}\frac{1}{S^{+2}}-50.22+v_{av}^{+}+F(30) \quad (\theta=\frac{\pi}{2}) \tag{4.4.8'}$$

$(5\leqq S^{+}\leqq 30)$

$$\frac{1}{S_t^{+}} = 5\ln\frac{25.205}{S^{+}-4.795}+v_{av}^{+}-13.25+F(30) \tag{4.4.9}$$

$(30\leqq S^{+})$

$$\frac{1}{S_t^{+}} = v_{av}^{+}-3.8-\frac{1}{0.36}\ln S^{+}+F(S^{+}) \tag{4.4.10}$$

and

$$F(x) = \frac{1}{0.36}\ln[\frac{R^{+}-x}{R^{+}-\exp\{0.36(v_{av}^{+}-3.8)\}}] \tag{4.4.11}$$

where,

$R^+ = R * u^* / \nu$

$u^* = (f/2)^{(1/2)} * v_{av}$

$u_t = \rho_p * D_p^2 * g / (18\mu)$

$v_{av}^+ = v_{av} / u^*$

where, R^+ (-) is the dimensionless radius of the pipe, S_t^* (-) the Stokes number, u^* (m/s) the representative flow velocity involving a fraction of a duct, u_t (m/s) the gravitational deposition rate, v_{av}^+ (-) the dimensionless average velocity of the fluid, v_{av} (m/s) the average velocity in a duct. θ (-) is the angle from the vertical axis, μ (kg/m·s) the viscosity, ν (m^2/s) the kinematic viscosity of fluid and ρ_p (kg/m^3) the density of aerosol particles.

3) Thermophoretic deposition of aerosol

The deposition rate of aerosol particles due to the thermophoretic, v_T, is given by Jacobsen-Brock's equation[13], as follows:

$$V_T = Z_T \cdot \left(- \frac{dT}{dn}\right) \tag{4.4.12}$$

$$Z_T = \frac{3 \cdot \nu \{\lambda_g + C_t \cdot Kn \cdot \lambda_p + 4 \cdot b \cdot C_m \cdot Kn(\lambda_g + C_t \cdot Kn \cdot \lambda_p - \lambda_p)/3\}}{2 \cdot T(1 + 3 \cdot C_m \cdot Kn)(2\lambda_g + \lambda_p + 2 \cdot C_t \cdot Kn \cdot \lambda_p)} \tag{4.4.13}$$

where, b (=2.4), C_m (=1.0) and C_t (=3.32) are correction coefficients. Kn (-) is the Knudsen number, n (m) the boundary layer on the deposition surface, T (K) absolute temperature of gas phase. λ_g (J/m·s·K) and λ_p (J/m·s·K) are the heat conductance of gas and aerosol. ν (m^2/s) is the kinematic viscosity of gas.

The temperature gradient (dT/dn) at the boundary layer between the gas phase and duct wall on the deposition surface is obtained by the following equation:

$$\frac{dT}{dn} = - \frac{Nu}{D_a}(T_g - T_w) \tag{4.4.14}$$

where, D_a (m) is the diameter of the duct, Nu (-) the Nusselt number, T_g (K) the gas phase temperature and T_w (K) is the temperature on the inner wall of the duct.

(2) Deposition of aerosol in the cell

1) Diffusional deposition in the cell

The diffusional deposition rate of the aerosol on the cell wall, v_D, is calculated by the Stokes-Einstein's equation.

$$v_D = \frac{D_s}{\delta_g} \tag{4.4.15}$$

$$D_s = \frac{k \cdot T}{f_a} \tag{4.4.16}$$

$$f_a = \frac{2}{3} D_p^2 \cdot \rho_g \left(\frac{2 \cdot \pi \cdot k \cdot T}{m_a}\right)^{(1/2)} \left(1 + \frac{0.9\pi}{8}\right) \tag{4.4.17}$$

where, D_s (m^2/s) is the diffusion coefficient of aerosol, D_p (m) the diameter of aerosol, f_a (kg/s) the friction coefficient of the fluid, m_a (kg) the mass of gaseous molecule ($=4.81564 \times 10^{-26}$), T (K) the absolute temperature of gas, δ_g (m) the thickness of boundary layer between the gas phase and cell wall and ρ_g (kg/m^3) the density of gas.

2) Gravitational deposition of aerosol

Gravitational deposition of aerosol in the cell, v_a, is calculated by Stokes's equation, as follows:

$$v_s = \frac{2(\rho_p - \rho)}{9 \cdot \mu} R_p^2 \cdot g \ (1 + A_k \cdot Kn) \tag{4.4.18}$$

where, R_p (m) is the radius of aerosol, A_k (-) the slip-factor, g (m/s^2) the gravitational acceleration, Kn (-) the Knudsen number, ρ (kg/m^3) the density of air, ρ_p (kg/m^3) the density of the aerosol and μ (kg/m·s) the viscosity.

$$A_k = 1.25 + 0.42 \exp\left(\frac{-0.87}{Kn}\right) \tag{4.4.19}$$

$$Kn = \frac{l}{R_p} \tag{4.4.20}$$

$$l = \nu \left(\frac{0.029}{6 \cdot 10^{23}} \cdot \frac{\pi}{2 \cdot k \cdot T}\right)^{0.5} \qquad (4.4.21)$$

where, l is the molecular mean free path of air, k the Boltzmann constant and ν the kinematic viscosity.

3) Temperature gradient at the thermophoretic deposition layer in the cell

The thermophoretic deposition rate of aerosol in the cell, v_T, is obtained by Jacobsen-Brock's equation[13] expressed in Eq.(4.4.12).

The temperature gradient (dT/dn) in Eq.(4.4.12) is given by Eq.(4.4.22).

$$\frac{dT}{dn} = -\frac{\alpha_c}{\lambda_g}(T_g - T_w) \qquad (4.4.22)$$

where, α_c (J/m^2·s·K) is the heat transfer coefficient obtained from the Nusselt number expressed in Chap. 4.3.2.(3). λ_g (J/m·s·K) is the heat conductivity of gas, T_g (K) the gas temperature, and T_w (K) the temperature of the inner wall.

4.4.3 Calculation of the HEPA filter

Aerosols generated by a solvent fire or an explosion are transferred through the cells and ducts, adhering to walls due to depositions, and collected by the HEPA filter at the end of the ventilation system. Clogging by generated smoke will affect the integrity of the HEPA filters.

(1) Differential pressure across the HEPA filter

The differential pressure across the HEPA filter clogging by smoke is obtained by the flow rate of fluid through the filter, as follows:

$$\Delta P_o = a \cdot Q + b \cdot \rho \cdot Q^2 \qquad (4.4.23)$$

where, Q (m^3/s) is the volume flow rate through the filter in the ventilation system, ρ (kg/m^3) the density of the fluid. a and b are the empirical coefficients obtained by the solvent fire tests. In Eq.(4.4.23), first term is for the laminar and second term for the turbulent flow rate of fluid through the filter. ΔP_o by Eq.(4.4.23) is used in Eq.(3.1.3). Table 4.4 shows the

laminar flow resistance coefficient, K_L ($m^{-1/2}$), and turbulent flow resistance coefficient, K_T(-), for new the HEPA filter. K_L and K_T are not effected by the number of filters.

(2) Efficiency of aerosol collection by the HEPA filter

The efficiency of aerosol collection by the HEPA filter is expressed as a decontamination factor, DF, which is defined by concentrations of aerosol after and before the filter. The user can set for input of DF_i corresponding to the i-th class aerosol in a particle size distribution.

The aerosol weight collected by the HEPA filter is obtained by the following equation, using efficiency ($E_{f,i}$) for the i-th particle.

$$\frac{dL_{so}}{dt} = Q \cdot \sum_i E_{f,i} \cdot C_i \qquad (4.4.24)$$

where, L_{so} (kg) is the weight of aerosol loaded on the filter, C_i (kg/m^3) the concentration of the ith-particle before the filter, Q (m^3/s) the volume flow through the filter. The efficiency, $E_{f,i}$, of the i-th particle is expressed by DF_i, as follows:

$$E_{f,i} = (1 - \frac{1}{D \cdot F_i}) \qquad (4.4.25)$$

The aerosol weight collected on the filter, L_s, is obtained by Eq.(4.4.26), using the number of the filter as N.

$$L_s = \frac{L_{so}}{N} \qquad (4.4.26)$$

(3) Flow resistance of the HEPA filter clogged by smoke

The flow resistance caused by aerosol loading onto the HEPA filter, ΔP (Pa), is given by Eq.(4.4.27) which is expressed in Appendix 4.

$$\Delta P = \Delta P_o \ (1 + \alpha \cdot L_s + \beta \cdot L_s^2) \qquad (4.4.27)$$

where, ΔP_o (Pa) is the pressure difference across the new filter in Eq.(3.1.3), L_s (kg/(unit filter)) the aerosol weight loading per one-unit filter. α and β are determined by the solvent fire tests[6] in JAERI.

1) Loading of smoke

Due to the smoke during a solvent fire, the differential pressure of a HEPA filter is increased due to clogging. The differential pressure is proportional to the amount of the burning solvent in the cell, because the generation of smoke is proportional to the burning rate of solvent as shown in Appendix 4. The differential pressure due to the smoke clogging, P_s (-), is calculated, as follows:

$$P_s = 1 + 12.23L_s + 28.79L_s^2 \quad (4.4.28)$$

2) Loading of a wetted aerosol

A radioactive wetted aerosol is generated by an explosion. The wetted aerosol changes to a dried one due to the heat of the explosion, which is explained in Chap. 4.2.3 (3). For clogging by a wetted aerosol, the empirical equation for the differential pressure, P_s (-), is obtained, as follows[15]:

$$P_s = 1 + 12.4L_s + 44.67L_s^2 \quad (4.4.29)$$

3) Loading of a dried aerosol

The differential pressure across the filter caused by a dried aerosol may be considered to be small in comparison with the cause of a wetted aerosol. The measurement of HEPA filter clogging by a dried aerosol was determined by a clay aerosol of JIS11-dust[15]. The differential pressure, P_s (-), is obtained by Eq.(4.4.30).

$$P_s = 1 + 1.26L_s + 0.446L_s^2 \quad (4.4.30)$$

Those from Eqs.(4.4.28) to (4.4.30) are empirical equations obtained from the experiments under a constant flow rate condition.

4.5 Other added functions

4.5.1 Automatic openning and shutting for a relaxation valve

This is a function of an automatic openning and shutting-type valve, which is moved by monitoring the signals of the pressure or flow rate at any node and branch in the ventilation system.

(1) Control by pressure signal

For the control of relaxation valve, the users must set a fixed pressure, P_o (Pa), and a pressure width, ΔP (Pa), for the monitoring node as the input. New cross-sectional area of the valve is determined by the following equation:

$$S_v(t+\Delta t) = S_v(t) \pm S_{vo} \cdot f_v \cdot \Delta t \qquad (4.5.1)$$

where, $S_v(t)$ (m^2) is the cross-sectional area of the valve at the time t, S_{vo} (m^2) the maximum cross-sectional area, f_v (%/s) the openning or closing rate of the valve, and Δt (s) the time step, respectively. The term of $[S_{vo} \cdot f_v \cdot \Delta t]$ means the change in the cross-sectional area of the valve at time interval Δt. If the variation of pressure in the node is detected smaller than the preset pressure width of ΔP, the valve change speed becomes slower with a small value of f_v. On the other hand, if the variation is larger than ΔP, the speed becomes fast with a big value of f_v.

(2) Control by flow rate signal

A fixed flow rate, Q (m^3/s), and a flow rate width of ΔQ (m^3/s) must be determined by users for the monitoring branch. A new cross-sectional area, $S_v(t+\Delta t)$ (m^2), is also determined by the similar equation of Eq.(4.5.1). If variation of the flow rate is smaller than the input flow rate width ΔQ, the valve moves slowly, if the flow rate variation is larger than ΔQ, the valve speed becomes fast.

4.5.2 Automatic control of check valve

In the fuel reprocessing plant, check valves are equipped in the ventilation system to prevent a back flow of fluid through the valve from the cell to outside of the cell. TRANS-ACE has the function of automatic addition and control of the check valve at the boundary point in the ventilation system. Figure 4.3 shows the schematic of the check valve. In this case, the branch number of the added check valve and node number of the added new node in Figure 4.3 are defined as last number of the branches and nodes in the ventilation system, respectively.

4.5.3 Automatic time step setting

This is a function of time step setting in the calculation by TRANS-ACE. If the variation of physical values calculated is large, the time step becomes shorter automatically, but if small, the time step becomes larger.

Variation ratio, E, of a certain physical value such as pressure, density or flow rate at the time interval Δt is obtained by the following equation:

$$E_1 = \frac{f(t+\Delta t)-f(t)}{f(t)} \tag{4.5.2}$$

where, f(t) is the time function of the physical value.

In TRANS-ACE, the second derivative equation is also programmed.

$$E_2 = \frac{\alpha(t+\Delta t)-\alpha(t)}{\alpha(t)} \tag{4.5.3}$$

$$\alpha = f(t+\Delta t)-f(t) \tag{4.5.4}$$

Time step is automatically set by the comparison between the E (E_1 or E_2) and MAXV or MINV. MAXV and MINV are maximum and minimum values of the variation ratio of the physical quantities, respectively. They are given by the input data. If one of the physical quantities such as pressure, density and flow rate is out of the region between MAXV AND MINV, the time step is set automatically. In this judgment, there is no priority among the physical quantities. E_2 is set to be 2.0 in the subroutine program "AUTOSTP".

This function has not completed yet. So it is necessary to improve the program of TRANS-ACE.

Table 4.1 Burning Parameters for Solvent Fire

Symbol	Phenomenon	Definition	Empirical equation
ξ	Efficiency of a solvent burning	$\frac{\text{Burning rate of a solvent}}{\text{Mass loss rate of a solvent}}$	$\xi = \frac{m_b}{[m_{fu}]_A}$ =1.0(Fire under atmosphere) =exp[0.889ln(F/S)+1.175](F/S≦2) =exp[0.128ln(F/S)-0.268](F/S>2)
ε	Heat accumulation in a burning pan	$\frac{\text{Heat flow due to a solvent vaporization}}{\text{Heat flow from flalme to a burning pan}}$	$\varepsilon = \frac{[m_{fu}]_A \cdot L_{fu}}{[q]_{x=0}}$ =0.3～0.4
ϕ	Radiation to a burning pan	$\frac{\text{Heat flow into pool due to radiative effect}}{\text{Heat flow from a flame to a burning pan}}$	$\phi = \frac{[q_r]_A}{[q]_{x=0}}$ =0.85-0.46exp(-4.2d)
γ	Total radiative effects to a wall	$\frac{\text{Total heat flow due to radiative effects}}{\text{Total heat generation due to a burning}}$	$\gamma = \frac{[q]_A+[-q]_B}{m_b \Delta H}$=0.15
f	Effect of solvent burning by oxygen	$\frac{\text{Burning rate of the solvent}}{\text{Oxygen rate needed to burn a solvent}}$	$f = \frac{\xi [m_{fu}]_A}{[-m_{fu}]_B}$ =0.288(n-dodecane) =0.333(30%TBP/n-dodecane)
δ	Effect of water boiling	$\frac{\text{Mass loss rate of water}}{\text{Mass loss rate of solvent}}$	$\delta = \frac{[m_{aq}]_A}{[m_{fu}]_A}$ =0.1(Fire under atmosphere) =0.0(Fire in cell)
Y_{ox}	Effect of oxygen	$\frac{\text{Oxygen concentration difference between}}{\text{infinite position and a flame}}$	Y_{ox} =0.232(Fire under atmosphere) =0.232exp[-28.8(V_f/V_L)](fire in cell)

Table 4.2 Amounts of Radioactive Materials at Extraction Process of a Large-scale Fuel Reprocessing Plant (Cooling time : 4 (years), burn-up : 45 (GWD/tU), initial enrichment : 4.5 (%))

Nuclide	Activity (Ci)	Concentration (Ci/l)	Distribution coefficient(-)	Entrainment coefficient(-)
^{3}H	5.8×10^{-4}	1.2×10^{-1}	2.0×10^{-3}	1.0×10^{0}
^{90}Sr	9.2×10^{-2}	1.8×10^{1}	5.0×10^{-4}	3.0×10^{-3}
^{90}Y	9.2×10^{-2}	1.8×10^{1}	2.0×10^{-4}	3.0×10^{-3}
^{106}Ru	4.1×10^{-2}	8.1×10^{0}	3.0×10^{-2}	1.0×10^{-1}
^{106}Rh	4.1×10^{-2}	8.1×10^{0}	1.0×10^{-5}	1.0×10^{-2}
^{125}Sb	6.3×10^{-3}	1.3×10^{0}	1.0×10^{-5}	1.0×10^{-2}
^{125m}Te	1.5×10^{-3}	3.1×10^{-1}	1.0×10^{-5}	1.0×10^{-2}
^{134}Ce	6.3×10^{-2}	1.3×10^{1}	8.0×10^{-5}	1.0×10^{-1}
^{137}Ce	1.3×10^{-1}	2.6×10^{1}	8.0×10^{-5}	1.0×10^{-1}
^{137m}Ba	1.2×10^{-1}	2.4×10^{1}	1.0×10^{-4}	1.0×10^{-3}
^{144}Ce	3.7×10^{-2}	7.5×10^{0}	1.0×10^{-2}	1.0×10^{-3}
^{144}Pr	3.7×10^{-2}	7.5×10^{0}	1.0×10^{-5}	1.0×10^{-3}
^{144m}Pr	5.0×10^{-4}	9.0×10^{-2}	1.0×10^{-5}	1.0×10^{-3}
^{147}Pm	5.1×10^{-2}	1.0×10^{1}	1.0×10^{-2}	1.0×10^{-3}
^{151}Sm	5.0×10^{-4}	9.0×10^{-2}	1.0×10^{-5}	1.0×10^{-3}
^{154}Eu	5.7×10^{-3}	1.1×10^{0}	1.0×10^{-2}	1.0×10^{-3}
Uranium	2.0×10^{-6}	4.0×10^{-4}	4.0×10^{0}	5.0×10^{-4}
Plutonium	1.4×10^{-1}	2.8×10^{1}	1.0×10^{0}	5.0×10^{-4}
Actinium	4.4×10^{-3}	8.8×10^{-1}	2.0×10^{-1}	5.0×10^{-4}

Table 4.3 Amounts of Radioactive Materials at Extraction Process of a Small-scale Fuel Reprocessing Plant (Cooling time : 180 (days), burn-up : 25 (GWD／tU), initial enrichment : 4.5 (%))

Nuclide	Activity (Ci)	Concentration (Ci/l)	Distribution coefficient(-)	Entrainment coefficient(-)
^{89}Sr	1.53×10^{-1}	1.91×10^{1}	1.0×10^{-3}	3.0×10^{-3}
^{90}Sr	1.02×10^{-1}	1.27×10^{1}	1.0×10^{-3}	3.0×10^{-3}
^{137}Ce	9.60×10^{-2}	1.20×10^{1}	1.0×10^{-4}	1.0×10^{-1}
^{103}Ru	5.84×10^{-2}	7.30×10^{0}	1.0×10^{-2}	1.0×10^{-1}
^{106}Ru	4.18×10^{-1}	5.22×10^{1}	1.0×10^{-2}	1.0×10^{-1}
^{106}Rh	4.18×10^{-1}	5.22×10^{1}	1.0×10^{-3}	1.0×10^{-1}
^{95}Zr	2.64×10^{-1}	3.30×10^{1}	1.0×10^{-1}	1.0×10^{-1}
^{95}Nb	5.57×10^{-1}	6.96×10^{1}	1.0×10^{-2}	1.0×10^{-1}
^{141}Ce	3.20×10^{-2}	4.00×10^{0}	1.0×10^{-3}	5.0×10^{-4}
^{144}Ce	1.06×10^{0}	1.32×10^{2}	1.0×10^{-3}	5.0×10^{-4}
^{144}Pr	1.06×10^{0}	1.32×10^{2}	1.0×10^{-5}	5.0×10^{-4}
^{3}H	2.24×10^{-4}	2.80×10^{-2}	2.7×10^{-3}	1.0×10^{-1}
^{90}Y	1.02×10^{-1}	1.27×10^{1}	1.0×10^{-2}	3.0×10^{-3}
^{91}Y	2.22×10^{-1}	2.78×10^{1}	1.0×10^{-2}	3.0×10^{-3}
^{140}Ba	1.12×10^{-4}	1.40×10^{-2}	1.0×10^{-4}	3.0×10^{-3}
^{140}La	1.12×10^{-4}	1.40×10^{-2}	1.0×10^{-2}	5.0×10^{-4}
^{147}Pm	3.62×10^{-1}	4.50×10^{1}	1.0×10^{-2}	5.0×10^{-4}
Uranium	4.10×10^{-7}	5.10×10^{-5}	4.0×10^{0}	5.0×10^{-4}
Plutonium	6.40×10^{-4}	8.00×10^{-2}	1.0×10^{0}	5.0×10^{-4}

Table 4.4 Flow Resistance Coefficients of the HEPA filter

	Half-size (610mm×305mm×292mm)	Full-size (610mm×610mm×292mm)
K_L ($m^{-1/2}$)	9.986×10^{6}	9.953×10^{6}
K_T (－)	40.3	40.5

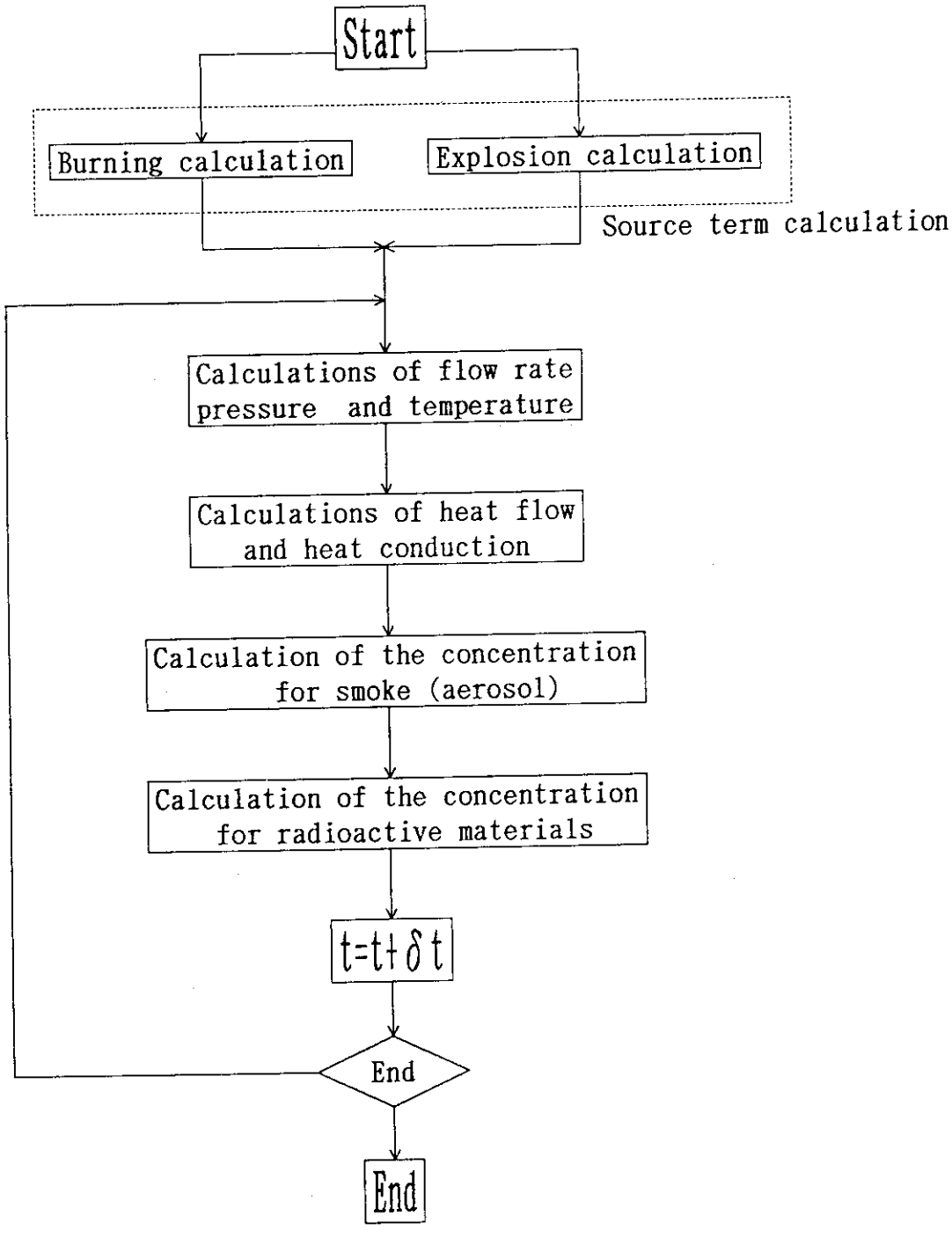

Fig. 4.1 Flow chart of fire and explosion conditions calculation.

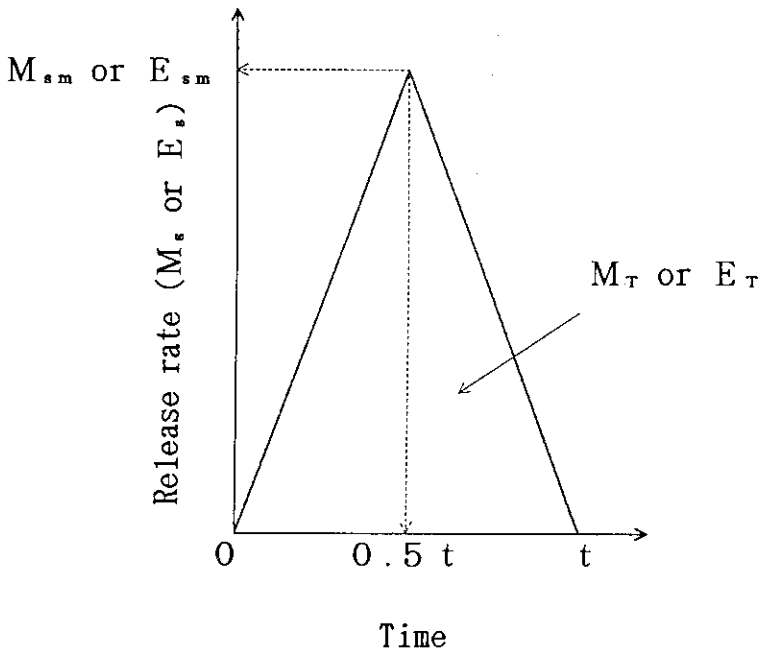

Fig. 4.2 Simple triangular spike of energy or mass source.

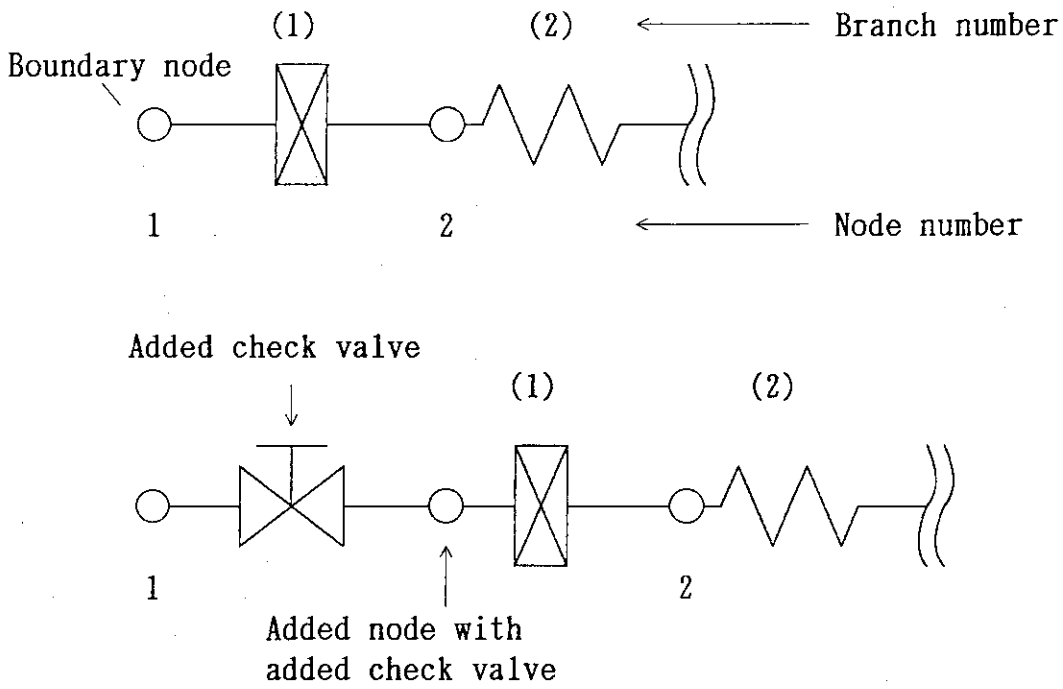

Fig. 4.3 Explanation of setting the back current check valve.

5. INPUT AND OUTPUT

5.1 Description of input

5.1.1 Contents of input cards

(1) Calculation control card

1. Title card
2. Simulation control card
3. Run control card
4. Time step card (1)
5. Time step card (2)
6. Time step card (3)
7. Calculation results output time control card

(2) Calculation parameter input card

1) Ventilation system data input card

8. Constitution of the ventilation system input card
9. Check valve automatic setting card
10. Flow resistance calculation control card

2) Accident control card

11. Accident condition setting card
12. Burning parameters input card
13. Solvent fire calculation data card (1)
14. Solvent fire calculation data card (2)
15. Explosion calculation data card (1)
16. Explosion calculation data card (2)
17. Aerosol data card (1)
18. Aerosol data card (2)
19. Aerosol data card (3)
20. Aerosol data card (4)
21. Aerosol data card (5)
22. Radioactive nuclides data card (1)
23. Radioactive nuclides data card (2)

3) Branch data card

24. Common branch data card (1)
25. Common branch data card (2)
26. Branch data card (1)

27. Branch data card (2)
28. Branch data card (3)
29. Blower characteristic data card (1)
30. Blower characteristic data card (2)
31. Filter flow resistance input card
32. Filter collection efficiency input card (1)
33. Filter collection efficiency input card (2)
34. Filter collection efficiency input card (3)
35. Filter collection efficiency input card (4)

4) Node data card
36. Boundary node data card
37. Common volume node data card (1)
38. Common volume node data card (2)
39. Time function control card
40. Volume node data card (1)
41. Volume node data card (2)
42. Volume node data card (3)
43. Volume node data card (4)
44. Node initial pressure data card
45. Node initial temperature data card
46. Node initial aerosol data card
47. Time function input data card (1)
48. Time function input data card (2)

5) Valve control data card
49. Valve control card (1)
50. Valve control card (2)
51. Valve control card (3)
52. Check valve automatic addition control card
53. Check valve automatic addition data card (1)
54. Check valve automatic addition data card (2)

6) Flow resistance automatic calculation card
55. Flow resistance automatic calculation data card (1)
56. Flow resistance automatic calculation data card (2)
57. Flow resistance of valve automatic calculation data card
58. Flow resistance of duct automatic calculation data card

7) Other physical property data card
59. Condition of atmosphere
60. Physical properties of fluid data card (1)
61. Physical properties of fluid data card (2)

(3)Output format control card
62. Plot control data card (1)
63. Plot control data card (2)
64. Plot control data card (3)
65. Plot control data card (4)

5.1.2 Formats of input cards
(1)Calculation control cards
1. Title card

Column number	40	
Data type	10A4	
Variable name	(Example) SOLVENT FIRE ACCIDENT	
Unit	-	

Comments in this card will be written on the output lists.

2. Simulation control card

Column number	5	
Data type	I5	
Variable name	NOPT1	
Unit	-	

NOPT1 is a selecting flag whether input data are checked or not.

3. Run control card

Column number	5 10			15	25	35	45	50	60	
Data type	X3	A2	X5	I5	F10.5	F10.5	F10.5	I5	F10.5	
Variable name		RUNT		MAXIT	CONVRG	RBETA	FMIX	MAXIT2	CONV2	
Unit		-		-	-	-	-	-	-	

RUNT is a selecting flag for calculation mode.
RUNT=SS: Steady state calculation, =RS: restart calculation
=ST: Accidental condition calculation
=SP: Steady state calculation (output to restart file)
=RP: Accidental condition calculation (output to restart file)
MAXIT : Maximum iteration times (default:1000)
CONVERG: Convergence judgment value (default:0.005)
RBETA : Easement coefficient (default:1.0)
FMIX : Mixing coefficient (default:0.77777)
MAXIT2 : Maximum iteration times at the initial steady loop (default:200)
CONV2 : Convergence judgment value at the initial steady loop (default:0.001)

4. Time step card (1)

Column number	5	15	25	35	45	
Data type	I5	F10.0	F10.0	F10.0	F10.0	
Variable name	IASTFG	MAXV	MINV	MAXT	MINT	
Unit	-	-	-	s	s	

IASTFG=0: Divided time step, =1: automatic time step
MAXV: Maximum value of $(f(t+\Delta t)-f(t))/f(t)$
MINV: Minimum value of $(f(t+\Delta t)-f(t))/f(t)$
MAXT: Maximum value of time step, MINT: minimum value of time step

5. Time step card (2)

Column number	10	~	60	
Data type	F10.5	~	F10.5	
Variable name	TSTCHG(1)	~	TSTCHG(6)	
Unit	s	~	s	

Changing time of time division are set.
TSTCHG(n): Changing time of the n-th time division (n=1~6)

6. Time step card (3)

Column number	10	~	70	
Data type	F10.5	~		
Variable name	TSTEP(1)	~	TSTEP(7)	
Unit	s	~	s	

Time steps corresponding to the time divisions are set.
TSTEP(n): Time step in the n-th time division

7. Calculation results output time control card

Column number		5	15	25	35	45	
Data type	X4	A1	F10.5	F10.5	F10.5	F10.5	
Variable name		NSOUT	SOUT(1)	SOUT(2)	SOUT(3)	CHEK	
Unit		-	s	s	s	s	

NSOUT is the number of output of the calculation results (default=0, maximum=3). The calculation results at the time of SOUT(n) are outputted to the output list. The result at the initial state and calculation results at the end are always outputted.
SOUT(n): Output time (n=0～NSOUT)
CHEK : Check time of the number of outputs

(2) Calculation parameter input card
1) Ventilation system data input card
8. Constitution of the ventilation system input card

Column number		5	10	15	20	25	30
Data type	I5	I5	I5	I5	I5	I5	
Variable name	N1	N2	N3	N4	N5	ISTACK	
Unit	-	-	-	-	-	-	

N1: Number of branches (≦200)
N2: Number of boundary nodes (≦10)
N3: Number of volume nodes (≦200)
N4: Number of blower property data table (≦20)
(Blower property is given in card-29～30)
N5: Number of filter property data table (≦50)
(Filter property is given in card-31)

9. Check valve automatic setting card

Column number		5
Data type	I5	
Variable name	IGYA	
Unit	-	

IGYA=0: Check valves are set automatically.
=1: Check valves are not set.

10. Flow resistance calculation control card

Column number	5	
Data type	I5	
Variable name	IDCAL	
Unit	-	

IDCAL=0: Initial flow resistance of the ventilation system is set by the user's input.
IDCAL=1: Initial flow resistance of the ventilation system is obtained by the automatic calculation.
IDCAL must be made 1 when IGYA is 1 in card-9.

(2) Accident control card
11. Accident condition setting card

Column number	5	10	15	25	
Data type	I5	I5	I5	E10.0	
Variable name	PHENOM	ICALT	IBROOM	HCELL	
Unit	-	-	-	m	

PHENOM=0: Source term is set by user as the time function in card-47.
=1: Source term is calculated by the automatic calculation function (solvent fire)
=2: Source term is calculated by the automatic calculation function (explosion)
ICALT =0: Heat release to the cell wall is not calculated.
=1: Heat release to the cell wall is calculated.
IBROOM : Node number of the accident cell
HCELL : Height of the accident cell

12. Burning parameters input card

Column number	10	20	30	40	50	
Data type	E10.0	E10.0	E10.0	E10.0	E10.0	
Variable name	GZAI	OXM	PSAI	EPS	GAMB2	
Unit	-	-	-	-	-	

Burning parameters are set. If these parameters are not set, they will be calculated by use of empirical equations in the code.

13. Solvent fire calculation data card (1)

Column number	10	20	30	40	50	
Data type	E10.0	E10.0	E10.0	E10.0	E10.0	
Variable name	QINT	DZPAN	BAREA	VTBP	VLS0	
Unit	m^3/s	m	m^2	-	m^3	

This card is read in case of PHENOM=1.
QINT : Air flow to the accident cell
DZPAN: Depth of burning pan in accident cell
BAREA: Burning area
VTBP : Volume fraction of TBP in a mixed solvent
VLS0 : Initial volume of a mixed solvent

14. Solvent fire calculation data card (2)

Column number	10	20	30	40	50	
Data type	E10.3	E10.3	E10.3	E10.3	E10.3	
Variable name	CPD	PR	VMID	TSS	TAD	
Unit	J/kg	-	kg/ms	s	K	

This card is read in case of PHENOM=1.
CPD : Specific heat of burning gas
PR : Plantdl number of burning gas
VMID: Viscosity coefficient of burning gas
TSS : Time of combustion extend to the steady state
TAD : Temperature at infinite position in cell

15. Explosion calculation data card (1)

Column number	10	15	
Data type	E10.0	I5	
Variable name	GRM	NTYPE	
Unit	kg	-	

This card is read in case of PHENOM=2.
GRM : Weight of explosive material
NTYPE=1: TNT, =2: red oil, =3: hydrogen, =4: acetylene

16. Explosion calculation data card (2)

Column number	10	10	10	10	
Data type	E10.0	E10.0	E10.0	E10.0	
Variable name	SMOKEM	DMH2O	DOH2O	WRAD	
Unit	kg	kg	kg/m³	kg/m³	

This card is read in case of PHENOM=2.
SMOKEM: Weight of generated aerosol except for liquid aerosol from combustive materials
DMH2O : Weight of generated liquid aerosol from a dispersed solution
DOH2O : Density of a solution
WRAD : Weight concentration of solutes in a solution

17. Aerosol data card (1)

Column number	5	
Data type	I5	
Variable name	ICALC	
Unit	-	

ICALC=0 : Aerosol transport is not calculated.
ICALC=1 : Aerosol transport is calculated.

18. Aerosol data card (2)

Column number	10	20	30	40	50	60	70	
Data type	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	
Variable name	ALFNU	PK	ROUP	RG	DG	FALF	CDELT	
Unit	-	W/mK	kg/m³	-	m	-	m	

This card is read in case of ICALC=1.
ALFNU: diffusion coefficient of aerosol (=1.7)
PK : Heat conductivity of aerosol
ROUP : Density of aerosol
RG : Geometric standard deviation of log-normal distribution of aerosol
DG : Geometric means particle diameter of aerosol
FALF : Correcting parameter for friction coefficient
CDELT: Boundary layer thickness of gradient of temperature at the cell wall

19. Aerosol data card (3)

Column number	5	10	
Data type	I5	I5	
Variable name	IBUN	IBN	
Unit	-	-	

This card is read in case of ICALC=1.
IBUN=0: Programed log-normal distribution is used.
IBUN=1: Voluntary distribution by user's input is used.
IBUN : Number of division of voluntary distribution (≦14)
Even if programmed distribution is used, IBN is need for passing to read card-20 and card-21.

20. Aerosol data card (4)

Column number	10	~	70	
Data type	E10.5	~	E10.5	
Variable name	DI(1)	~	DI(7)	
Unit	m	~	m	

This card is read in case of ICALC=1 and IBUN=1. The voluntary distribution of aerosol is set by this card and next card.
DI(n): Aerosol particle diameter in the n-th division of the voluntary distribution (n=1~IBN)

21. Aerosol data card (5)

Column number	10	~	70	
Data type	E10.5	~	E10.5	
Variable name	WT(1)	~	WT(7)	
Unit	-	~	-	

This card is read in case of ICALC=1 and IBUN=1.
WT(n): Weight fraction of aerosol in the n-th division of the voluntary distribution (n=1~IBN)

22. Radioactive nuclides data card (1)

Column number	5	10	20	30	40	
Data type	I5	I5	E10.3	E10.3	E10.3	
Variable name	IFPDT	LSTFL	CUO2	VWTR	RUGAS	
Unit	-	-	kg/m³	-	-	

Inventory of radioactive nuclides at extraction process are set.
IFPDT=0: User input
=1: Programmed inventory for nuclear fuel reprocessing plant
=2: Programmed inventory for small type plant
LSTFL : Branch number of final filter of ventilation system
CUO2 : Weight concentration of uranium in aqueous phase
VWTR : Volume of aqueous phase
RUGAS : Gasification rate of ruthenium (default=0.04)

23. Radioactive nuclides data card (2)

Column number	10	20	30	40	
Data type	E10.0	E10.0	E10.0	E10.0	
Variable name	RAD	RADCON	DIS	EF	
Unit	Bq/kgU	Bq/m³	-	-	

Inventories for 20 nuclides are set. Even if nuclides do not need 20, user will have to give 20 cards with dummy data.
RAD : Activity of nuclide per kg-uranium (only fire accident)
RADCON: Concentration of activity of nuclide
DIS : Distribution coefficient of nuclide (only fire accident)
EF : Entrainment coefficient of nuclide (only fire accident)

3) Branch data card

24. Common branch data card (1)

Column number	5	~	30	
Data type	I5	~	I5	
Variable name	NOPT(1)	~	NOPT(6)	
Unit	-	~	-	

If some branch data are in common, those branch data are set in the lump by use of this card and next card.
NOPT(n): Number of common data card
n=1: Initial volume flow
n=2: Initial temperature of ducts
n=3: Density of duct walls
n=4: Specific heat of duct walls
n=5: Thickness of duct walls
n=6: Thermal conductivity of duct walls

25. Common branch data card (2)

Column number	5	10	20	
Data type	I5	I5	E10.0	
Variable name	IS	IE	(values)	
Unit	-	-	(Respectively)	

This card must be set number of NOPT(n).
IS : First branch number in the common block
IE : End branch number in the common block
values: Branch data in the common block
n=1: Initial volume flow (m^3/s)
n=2: Initial temperature of ducts (°C)
n=3: Density of duct walls (kg/m^3)
n=4: Specific heat of duct walls (J/kg·K)
n=5: Thickness of duct walls (m)
n=6: Thermal conductivity of duct wall (W/m·K)

26. Branch data card (1)

Column number	5	10	15	25	35	40		45	55	65	75	
Data type	I5	I5	I5	E10.0	E10.0	X4	A1	X3	I2	E10.0	E10.0	E10.0	
Variable name	IB	IL	I2	D2	D3		CH1		I3	D4	D1	D5	
Unit	-	-	-	m^2	m		-		-	Pa	m^3/s	m^2	

Branch data of each branch is given in this card, card-27 and card-28. These branch data have priority over the common branch data.
IB : Branch number
IL : Node number of the upper node of branch-IB
I2 : Node number of the lower node of branch-IB
D2 : Cross-sectional area of branch-IB (When branch-IB is butterfly valve or gate valve, θ or l/d is set, respectively)
D3 : Length of branch-IB (in case of duct)
CH1: Kind of branch-IB
=BV: Butterfly valve, =GV: Gate valve, =F : Filter,
=B : Blower, =D : Duct
I3 : Table number of blower property data in card-29 and card-30 or filter flow resistance data in card-31
D4 : Initial flow resistance at branch-IB (If initial flow resistance of branch-IB is obtained by automatic calculation, D4 must be 0.0)
D1 : Initial volume flow at branch-IB
D5 : Maximum cross sectional area of branch-IB (in case of valve)
If branch-IB is gate valve, D5 must be the following number:
=1: 0.5 inch caliber, =2: 1.0 inch caliber, =3: 10.0 inch caliber

27. Branch data card (2)

Column number	10	20	30	40	50	60	70		
Data type	X8	I2	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	
Variable name		IDUCT	DANGLE	DCTDEL	DCTRHO	DUCTCP	RDCT	DTEMP	
Unit		-	angle	m	kg/m³	J/kg·K	W/m·K	°C	

IDUCT : Division number of the duct wall thickness for heat transfer calculation
DANGLE: Angle of duct (0°～90°)
DCTDEL: Thickness of duct wall
DCTRHO: Density of duct wall
DUCTCP: Specific heat of duct wall
RDCT : Thermal conductivity of duct wall
DTEMP : Initial temperature of duct wall

28. Branch data card (3)

Column number	5	10	15		
Data type	I5	I5	X3	I2	
Variable name	IFULFO	IHLFFO		IKLFO	
Unit	-	-		-	

IFULFO: Number of full-size filters
IHLFFO: Number of half-size filters
IKLFO : Number of empirical equation for variation of flow resistance of filter by clogging
=1: Unloaded filter
=2: Fire (cloggong by smoke)
=3: Explosion (clogging by humidity aerosol)
=4: Explosion (clogging by dry aerosol)
=5: Explosion (input of amount of loaded aerosol)

29. Blower characteristic data card (1)

Column number	5	10	
Data type	I5	I5	
Variable name	J	NP	
Unit	-	-	

This card is combined with card-30. They must have number N4 set in card-8.
J : Table number
NP: Number of combinations between the volume flow and flow resistance in card-30

30. Blower characteristic data card (2)

Column number	10	20	30	40	50	60	
Data type	F10.2	F10.2	F10.2	F10.2	F10.2	F10.2	
Variable name	XB	FXB	XB	FXB	XB	FXB	
Unit	m^3/s	Pa	m^3/s	Pa	m^3/s	Pa	

If number of combinations between XB and FXB are more than 3, this card is added as the same format.
XB : Volume flow
FXB: Flow resistance

31. Filter flow resistance input card

Column number	5	10	20	
Data type	I5	E10.4	E10.4	
Variable name	K	AKL	AKT	
Unit	-	$m^{-1/2}$	-	

Flow resistance coefficients of filters are set. This card is necessary upto number N5 in card-8.
K : Table number (≤ 20)
AKL: Laminar flow resistance coefficient
AKT: Turbulent flow resistance coefficient
If AKL=0.0 then AKL is calculated in the code and AKT is set to 0.0.

32. Filter collection efficiency input card (1)

Column number	5	
Data type	I5	
Variable name	IFIL	
Unit	-	

IFIL=0: Programmed filter collection efficiency is used.
IFIL=1: Filter collection efficiency is set by the user's input.
In case of IFIL=1, the relationship between aerosol diameter and filter efficiency is set in card-33 or card-34 and card-35 and card-36.

33. Filter collection efficiency input card (2)

Column number	10	~	70	
Data type	E10.5	~	E10.5	
Variable name	DID2(1)	~	DID2(7)	
Unit	m	~	m	

This card is read in case of IFIL=1.
DID2(n) : Aerosol diameter (n=1~IBN, IBN is set in card-19)
DIDI2(n): Must be set with the particle size from small to large

34. Filter collection efficiency input card (3)

Column number	10	~	70	
Data type	E10.5	~	E10.5	
Variable name	ETID2(1)	~	ETID2(7)	
Unit	-	~	-	

This card is read in case of IFIL=1.
ETID2(n): Filter collection efficiency corresponding to the aerosol diameter in card-33 (n=1~IBN)

35. Filter collection efficiency input card (4)

Column number	10	~	70	
Data type	E10.5	~	E10.5	
Variable name	ETID3(1)	~	ETID3(7)	
Unit	-	~	-	

This card is read in case of IFIL=1.
ETID3(n): Collection efficiency of second filter (n=1~IBN)

4) Node data card

36. Boundary node data card

Column number	5	15	20	30	35	45	50	
Data type	I5	F10.2	I5	F10.2	I5	F10.2	I5	
Variable name	IBNNR	PB	IBPFN	TB	IBTFN	CB	IBCFN	
Unit	-	PaG	-	°C	-	kg/m³	-	

If pressure, temperature and concentration of aerosol at a node will be varied then the variations are given by card-47 and card-48 as time tables.

IBNNR: Node number of boundary node
PB : Initial pressure at node-IBNNR (default: 0.0 PaG)
IBPFN: Table number of pressure at node-IBNNR
TB : Initial temperature at node-IBNNR (default: atmosphere)
IBTFN: Table number of temperatures at node-IBNNR
CB : Initial concentration of aerosol at node-IBNNR
IBCFN: Table number of concentrations of aerosol at node-IBNNR

37. Common volume node data card (1)

Column number	5	~	25	
Data type	I5	~	I5	
Variable name	NOPT(1)	~	NOPT(6)	
Unit	-	~	-	

If some node data about the cell wall are in common, these node data are set in the lump by use of this card and next card.

NOPT(n): Number of the common data
n=1: Thickness (m), n=2: Density (kg/m³), n=3: Specific heat (J/kg·K)
n=4: Thermal conductivity (W/m·K), n=5: Temperature (°C)

38. Common volume node data card (2)

Column number	5	10	20	
Data type	I5	I5	E10.0	
Variable name	IS	IE	(value)	
Unit	-	-	(Respectively)	

This card must be set number of NOPT in card-37.

IS: First node number in the common block
IE: End node number in the common block
values: Node data in the common block

39. Time function control card

Column number	5	10	15	20	25	
data type	I5	I5	I5	I5	I5	
Variable name	N1	N2	N3	N4	N5	
Unit	-	-	-	-	-	

Number of the time function tables in card-47 and card-48 are set in this card.
N1: Number of time function tables of the aerosol release rate
N2: Number of time function tables of the pressure variation
N3: Number of time function tables of the temperature variation
N4: Number of time function tables of the energy release rate
N5: Number of time function tables of the mass release rate

40. Volume node data card (1)

Column number	5	15	25	30	35	40	45	50	
Data type	I5	F10.2	F10.2	I5	I5	I5	I5	I5	
Variable name	I1	VOL	RFA	NOC	NOP	NOT	NOE	NOM	
Unit	-	m^3	m^2	-	-	-	-	-	

Data of all volume nodes are set in this card, card-41 and card-42. These cards are used in the lump. Volume node data in these cards have priority over common volume node data.
I1 : Node number
VOL: Volume of node-I1
RFA: Cross-sectional area of node-I1
NOC: Time function table number of the aerosol release rate
NOP: Time function table number of the pressure variation
NOT: Time function table number of the temperature variation
NOE: Time function table number of the energy release rate
NOM: Time function table number of the mass release rate
These time function tables are set in card-47 and card-48. If PHENOM (in Card-11) is 1 or 2, NOC~NOM must be set to 0.

41. Volume node data card (2)

Column number	10	20	30	
Data type	E10.0	E10.0	E10.0	
Variable name	REDOT	RMDOT	RCDOT	
Unit	W	kg/s	kg/s	

REDOT: Initial value of energy source in node-I1
RMDOT: Initial value of mass source in node-I1
RCDOT: Initial value of aerosol source in node-I1

42. Volume node data card (3)

Column number		10	20	30	40	50	60	
Data type	X8	I2	E10.0	E10.0	E10.0	E10.0	E10.0	
Variable name		NCELL	DELCEL	RHOCEL	CPCELL	RPCELL	TEMPCEL	
Unit		-	m	kg/m³	J/kg·K	W/m·K	°C	

NCELL : Division number of the region from accidental source to cell wall for heat transfer calculation to a cell wall.
(If NCELL≦2, heat transfer to a cell wall is not calculated.)
DELCEL : Thickness of the wall of node-I1
RHOCEL : Density of the wall of node-I1
CPCELL : Specific heat of the wall of node-I1
RPCELL : Thermal conductivity of the wall of node-I1
TEMPCEL: Temperature of the wall of node-I1

43. Volume node data card (4)

Column number		5		10		15	
Data type	X4	A1	X4	A1	X4	A1	
Variable name		PINP		TINP		CINP	
Unit		-		-		-	

PINP, TINP and CINP are setting flags for initial values of pressure, temperature and aerosol concentration at each node, respectively.
PINP: If initial pressure at each node is set by the user's input, flag P is set. (default: 0.0 PaG)
TINP: If initial temperature at each node is set by the user's input, flag T is set. (default: atmosphere)
CINP: If initial aerosol concentration is set by user's input, flag C is set.
If the initial flow resistance of the ventilation system is calculated by automatic calculation (IDCAL=1 in card-10) or given by the flow resistance of the branches (card-26), flag P must not be set.

44. Node initial pressure data card

Column number	15	~	60	
Data type	E15.8	~	E15.8	
Variable name	P(1)	~	P(4)	
Unit	PaG	~	PaG	

This card is read in case of PINP='P'. If n is larger than 4, this card is added with the same format. If IGYA=1 (in card-9), pressure data of the added volume nodes accompanied with addition of the check valves are also needed.
P(n): initial pressure of n-th node

45. Node initial temperature data card

Column number	15	~	60	
Data type	E15.8	~	E15.8	
Variable name	T(1)	~	T(4)	
Unit	˚C	~	˚C	

This card is read in case of TINP='T'. If n is larger than 4, this card is added with the same format. If IGYA=1 (in card-9), temperature data of added volume nodes accompanied with addition of the check valves are also needed.

T(n): Initial temperature of n-th node

46. Node initial aerosol data card

Column number	15	~	60	
Data type	E15.8	~	E15.8	
Variable name	C(1)	~	C(4)	
Unit	kg/m^3	~	kg/m^3	

This card is read in case of CINP='C'. If n is larger than 4, this card is added with the same format. If IGYA=1 (in card-9), aerosol concentration data of added volume nodes accompanied with addition of the check valves are also needed.

C(n): Initial aerosol concentration of n-th node

47. Time function input data card (1)

Column number	5	10	15	
Data type	I5	I5	I5	
Variable name	IFN(n)	INP(n)	IMT(n)	
Unit	-	-	-	

Time function tables of the aerosol release rate, pressure variation, temperature variation, energy release rate and mass release rate as source terms in the accidental cell are set by combining this card and the next card (PENOM=0). Number of the combinations of this card and the next card is set in card-39. The user must select one combination from the following three combinations for the source term input.

A. Mass release rate and energy release rate
B. Pressure variation and temperature variation
C. Temperature variation and mass release rate

The selection is specified by setting NOC~NOM in card-40.
IFN(n): Time function table number (n=N1~N5(in card-39))
INP(n): Number of combinations of time and physical values in card-48 (n=N1~N5(in card-39))
IMT(n): Time function table number of temperature variations (in case of combination C.) (n=N1~N5(in card-39))

48. Time function input data card (2)

Column number	10	20	~	50	60	
Data type	E10.0	E10.0	~	E10.0	E10.0	
Variable name	T(n,1)	FT(n,1)	~	T(n,1)	FT(n,3)	
Unit	s	Respectively	~	s	Respectively	

T(n,m) : Time (n=N1~N5(in card-39)), m=1~INP(n))
FT(n,m): Physical value (n=N1~N5(in card-39), m=1~INP(n))

5) Valve control data card

49. Valve control card (1)

Column number	5	10	
Data type	I5	I5	
Variable name	IFAOPT	IVALNO	
Unit	-	-	

IFAOPT: =0: Valve control off, =1: Valve control on
IVALNO: Branch number of the controlled valve
Even if IFAOPT=0, IVALNO is necessary for passing to read card-50 and card-51.

50. Valve control card (2)

Column number	5	10	20	25	35	45	50	55	
Data type	X5	I5	E10.5	X5	E10.5	E10.5	X5	I5	
Variable name		IQBRA	QFIX		POPEN	QOPEN		INDZ	
Unit		-	m^3/s		PaG	m^3/s		-	

This card is read in case of IFAOPT=1.
IQBRA: Branch number of the flow rate monitoring branch
QFIX : Standard flow rate at branch-IQBRA
POPEN: Pressure width of basis on standard pressure PSTOP
QOPEN: Flow rate width of basis on standard flow rate QFIX
INDZ : Node number of the pressure monitoring node

51. Valve control card (3)

Column number	5	10	20	25	35	40	45	55
Data type	X5	I5	E10.0	X5	E10.5	X5	I5	E10.0
Variable name		IFAVAL	FARATE		FAMIN		ISTOP	PSTOP
Unit		-	%/s		%/s		-	PaG

This card is read in case of IFAOPT=1.
IFAVAL: Branch number of controlled valve
FARATE: Variation rate of cross-sectional area of branch-IFAVAL
(Pressure or flow rate is in the variation width)
FAMIN : Variation rate of cross-sectional area of branch-IFAVAL
(Pressure or flow rate is out the variation width)
ISTOP : <0: Controlled by flow rate, >0: Controlled by pressure
PSTOP : Standard pressure at node-INDZ

52. Check valve automatic addition control card

Column number	5	15	25	35	45
Data type	I5	E10.0	E10.0	E10.0	E10.0
Variable name	NVALBR	BQOPEN	BFARTE	BFAMAX	BFAMIN
Unit	-	m^2/s	%/s	m^2	%/s

This card is read in case of IGYA=1 (in card-9). This card is used with card-53 and card-54.
NVALBR: Branch number of automatic added check valve
BQOPEN: Flow rate width of basis on standard flow rate QFIX
BFARTE: Variation rate of cross-sectional area of branch-NVALBR
(Flow rate is in the flow rate width)
BFAMAX: Maximum cross-sectional area of branch-NVALBR
BFAMIN: Variation rate of cross-sectional area of branch-NVALBR
(Flow rate is out the flow rate width)

53. Check valve automatic addition data card (1)

Column number	5	15	25	30	35	40	45	
Data type	I5	F10.2	F10.2	I5	I5	I5	I5	
Variable name	IWBNOD	DIFP	FA	IVALTP	ICARBR	ISLPD	ITHETA	
Unit	-	Pa	m^2	-	-	-	-	

This card is read in case of IGYA=1 (in card-9). Data of the automatic added check valve are set.

IWBNOD: Boundary node number of adding check valve-NVALBR
DIFP : Initial flow resistance at the check valve-NVALBR
FA : Cross-sectional area of the check valve-NVALBR
IVALTP: Type of the check valve-NVALBR
=0: Gate valve, =1: Butterfly valve
ICARBR: Caliber (ICARBR is set in case of IVALTP=0.)
=1: 1/2 caliber, =2: 1 caliber, =3: over 10 caliber
ISLPD : Degree of open of gate valve
=1: (l/d)=1/8, =2: (l/d)=1/4, =3: (l/d)=3/8
=4: (l/d)=1/2, =5: (l/d)=3/4, =6: (l/d)=1
ITHETA: Degree of open of butterfly valve
=1: (θ)= 5°, =2: (θ)=10°, =3: (θ)=20°, =4: (θ)=30°
=5: (θ)=40°, =6: (θ)=50°, =7: (θ)=60°, =8: (θ)=70°

54. Check valve automatic addition data card (2)

Column number	5	15	25	35	45	55	65	75	80	
Data type	I5	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	I5	
Variable name	IWBNOD	VOL	RFA	DELCEL	RHOCEL	CPCELL	RPCELL	TCEL	NCELL	
Unit	-	m^3	m^2	m	kg/m^3	J/kg°C	W/m°C	°C	-	

This card is read in case of IGYA=1 (in card-9). Data of automatic added node with addition of check valve-NVALBR.

IWBNOD: boundary node number of adding check valve-NVALBR
VOL : Volume of the added node
RFA : Cross-sectional area of the added node
DELCEL: Thickness of wall of the added cell
RHOCEL: Density of wall of the added cell
CPCCEL: Specific heat of wall of the added cell
RPCELL: Thermal conductivity of wall of the added cell
TCEL : Temperature of wall of the added cell
NCELL : Division number of the region for heat transfer calculation
(If NCELL≦2, heat transfer is not calculated.)

6) Flow resistance automatic calculation card

55. Flow resistance automatic calculation data card (1)

Column number	5	10	15	
Data type	I5	I5	I5	
Variable name	IERVAL	IVALCT	IDUCT	
Unit	-	-	-	

IERVAL: Number of error adjustment valves
IVALCT: Number of valves which initial flow resistance is set by the automatic calculation function
IDUCT : Number of ducts which initial flow resistance is set by the automatic calculation function

Even if IDCAL=0 (in card-10), IVALCT and IDUCT must set the number of combination of card-56 and card-57.

56. Flow resistance automatic calculation data card (2)

Column number	5	~	50	
Data type	I5	~	I5	
Variable name	IERVNO(1)	~	IERVNO(10)	
Unit		~		

IERVNO(n): Branch number of calculational error adjustment valve (n=1~IERVAL)

57. Flow resistance of valve automatic calculation data card

Column number	5	10	15	20	25	
Data type	I5	I5	I5	I5	I5	
Variable name	IDVALV	IVALTP	ICARBR	ISLPD	ITHETA	
Unit	-	-	-	-	-	

IDVALV: branch number of valve (Automatic calculation was done.)
IVALTP: =0: Gate valve, =1: Butterfly valve
ICARBR: Caliber (ICARBR is set in case of IVALTP=0.)
=1: 1/2 caliber, =2: 1 caliber, =3: over 10 caliber
ISLPD : Degree of open of gate valve
=1: (l/d)=1/8, =2: (l/d)=1/4, =3: (l/d)=3/8
=4: (l/d)=1/2, =5: (l/d)=3/4, =6: (l/d)=1
ITHETA: Degree of open of butterfly valve
=1: (θ)= 5°, =2: (θ)=10°, =3: (θ)=20°, =4: (θ)=30°
=5: (θ)=40°, =6: (θ)=50°, =7: (θ)=60°, =8: (θ)=70°

58. Flow resistance of ducts automatic calculation data card

Column number	5	10	20	30	40	
Data type	I5	I5	E10.0	E10.0	E10.0	
Variable name	IDDUCT	ILBO	RLBO	EPSRN	DCAL	
Unit	-	-	m	m	m	

IDDUCT: Branch number of duct (Automatic calculation was done.)
ILBO : =0: Elbo, =1: Not elbo
RLBO: Curvature of the elbo
EPSRN : Roughness coefficient
DCAL : Hydraulic diameter
(default: ((cross-sectional area)/π)$^{(1/2)}$)

7) Other physical properties data card
59. Condition of atmosphere data card

Column number	10	20	30	40	50	60	70	
Data type	E10.0	E10.0	E10.0	E10.0	E10.0	E10.0	E10.0	
Variable name	AMBBT	AMBCP	AMBRU	AMBKP	AMBMU	AMBTM	D1	
Unit	K^{-1}	J/kg·K	W/m·K	kg/m^3	Pa·s	°C	Pa	

AMBBT: Volume expansion coefficient of atmosphere
AMBCP: Heat capacity at constant pressure of atmosphere
AMBRU: Density of atmosphere
AMBKP: Thermal conductivity of atmosphere
AMBMU: Viscosity coefficient of atmosphere
AMBTM: Temperature of atmosphere, D1: Pressure of atmosphere

60. Physical properties of fluid data card (1)

Column number	10	20	30	40	50	60	70	
Data type	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	E10.5	
Variable name	ANU	XKAPA	ROU	CP	EPSH	AMU	AIRM	
Unit	m^2/s	J/m·s·K	kg/m^3	J/kg·K	m^2/s	K^{-1}	Pa·s	

ANU : Molecular kinematic viscosity coefficient
+ Vortex kinematic viscosity coefficient of fluid
XKAPA: Heat transfer coefficient of fluid
ROU : Density of fluid
EPSH : Vortex thermal conductivity of fluid
AMU : Volume expansion coefficient of fluid
AIRM : Molecular viscosity coefficient of fluid

61. Physical properties of fluid data card (2)

Column number	10	20	30	
Data type	E10.5	E10.5	E10.5	
Variable name	DINNU	VROOM	EMIT	
Unit	m^2/s	m/s	-	

DINNU: Kinematic viscosity coefficient of gas in duct
VROOM: Gas velocity near cell wall
EMIT : Radiation rate from gas phase to cell wall

(3) Out put format control card

62. Plot control data card (1)

Column number	5	10	15	20	25	30	35	40	45	50	
Data type	I5	I5	I5	I5	I5	I5	I5	I5	I5	I5	
Variable name	NPFRMS	NDPFRM	NTFRMS	NNWLIN	NNWLOT	NDWLIN	NDWLOT	NQFRMS	NMFRMS	NHFCIN	
unit	-	-	-	-	-	-	-	-	-	-	

If user does not need any graphs, the number of graphs is set 0.
NPFRMS: Number of graphs of the pressure at the nodes
NDPFRM: Number of graphs of the flow resistance at the branches
NTFRMS: Number of graphs of the temperature at the nodes
NNWLIN: Number of graphs of the temperature at the inner wall of the cells
NNWLOT: Number of graphs of the temperature at the outer wall of the cells
NDWLIN: Number of graphs of the temperature at the inner wall of the ducts
NDWLOT: Number of graphs of the temperature at the outer wall of the ducts
NQFRMS: Number of graphs of the volume flow at the branches
NMFRMS: Number of graphs of the mass flow rate at the branches
NHFCIN: Number of graphs of the heat flux to the inner wall of the cells

63. Plot control data card (2)

Column number	5	10	15	20	25	30	35	40	45	50	
Data type	I5	I5	I5	I5	I5	I5	I5	I5	I5	I5	
Variable name	NHFCOT	NHFDIN	NHFDOT	NARFRM	NCELDR	NDCTDR	NSDERF	NSMKDF	NCORAM	NRLRAM	
Unit	-	-	-	-	-	-	-	-	-	-	

If user does not need any graphs, the number of graphs is set 0.
NHFCOT: Number of graphs of the heat flux from the outer wall of the cells to atmosphere
NHFDIN: Number of graphs of the heat flux to the inner wall of the ducts
NHFDOT: Number of graphs of the heat flux from the outer wall of the ducts to atmosphere

NARFRM: Number of graphs of the aerosol concentration in the nodes
NCELDR: Number of graphs of the aerosol deposition rate in the cells
NDCTDR: Number of graphs of the aerosol deposition rate in the ducts
NSDEPF: Number of graphs of the aerosol deposition percentage
NSMKDF: Number of graphs of the integrated aerosol deposition and collection
NCORAM: Number of graphs of the radioactivity concentration at the stack
NRLRAM: Number of graphs of the radioactivity release rate at the stack

64. Plot control data card (3)

Column number	5	10	
Data type	I5	I5	
Variable name	IPLOT	ISCAL	
Unit	-	-	

IPLOT: =0: Output to line printer (LP)
=1: Output to plotter (NLP)
=2: Output to LP and NLP
ISCAL: =0: Y-axis is indicated as a percentage of the maximum value
=1: Y-axis is indicated as the maximum value
=2: Y-axis is indicated as a percentage and the maximum value
Default values of IPLOT and ISCAL are 0.

65. Plot control data card (4)

Column number	5		10	15	~	30	
Data type	A4	X1	I5	I5	~	I5	
Variable name	CHLOG(K)		NCRVS(K)	NCID(1,K)	~	NCID(4,K)	
Unit	-		-	-	~	-	

CHLOG(K) : =' ': Y-axis is indicated as linear.
='LOG': Y-axis is indicated as a logarithm.
NCRVS(K) : Number of plotted lines in one graph
NCID(n,K): Node or branch number of the n-th plotted line
(K=1~value defined in card-62 or card-63)

5.1.3 Example of input data setting

TRANS-ACE can evaluate various accident conditions with a combination of some of the programmed functions. An Example of the input data setting for the three cases are shown as follows.

(1) CASE-1

1) Accident : solvent fire
2) Source term option : automatic calculation
3) Heat transfer calculation to wall: on
4) Aerosol transport calculation : on (default distribution)
5) Initial flow resistance option : automatic calculation
6) Filter collection efficiency : default data
7) Automatic addition of check valve: on
8) Automatic open and shut of valve : on (pressure signal)
9) Time step : automatic time step

1),2) Flag PHENOM in Card-11 is made 1. Data for calculation of source term, burning parameters, shapes of nodes and physical properties, are given in Card-12, 13 and 14. NOC, NOP, NOT, NOE and NOM in Card-40 are made 0. In this case, even if the source terms are set as time function tables in Card-39, Card-47 and 48, they will be ignored.

3) Flag ICALT in Card-11 is made 1. Data for calculation of heat transfer are set in Card-25 or Card-27 (for branches) and Card-38 or Card-42 (for nodes).

4) Flag ICALC in Card-17 is made 1. Flag IBUN in Card-19 is made 0. Geometric average diameter and geometric standard deviation are given in Card-18.

5) Flag IDCAL in Card-10 is made 1. Flag D4 of the automatic calculating branches in Card-26 are made 0. Initial flow resistances of the branches which are set by the user's input are given as D4 directly. Flow resistances which are set by D4 have priority over the flow resistances which are calculated automatically.

6) Flag IFIL in Card-32 is made 0.

7) Flag IGYA in Card-9 is made 1. Flow resistances of added check valves are obtained by automatic flow resistance calculation.

8) Flag IFAOPT in Card-49 is made 1. Data of controlled valves are set in Card-50 and 51. When the added check valves are controlled, data of the added check valves are set in Card-52, 53 and 54.

9) Flag IASTFG in Card-4 is made 1. In this case, the time step in Card-6 is used initial value of automatic time step.

(2) CASE-2

1) Accident : solvent fire or explosion
2) Source term option : user's input
3) Heat transfer calculation to wall: off
4) Aerosol transport calculation : on (specified distribution)
5) Initial flow resistance option : user's input by node data
6) Filter collection efficiency : user's input
7) Automatic addition of check valve: on
8) Automatic open and shut of valve : on (flow rate signal)
9) Time step : divided time step

1),2) Flag PHENOM in card-11 is made 0. Mass release rate, energy release rate and aerosol release rate previously are specified by user as some time function tables in Card-47 and 48. User selects a combination of the source terms using card-40.
3) Flag ICALT in Card-11 is made 0.
4) Flag ICALC in Card-17 is made 1. Flag IBUN in Card-19 is made 1. Distribution of aerosol are specified in Card-20 and 21.
5) Flag IDCAL in Card-10 is made 0. Flag PINP in Card-43 is made "P" and pressures at respective nodes are given in Card-44. If initial flow resistances of some branches are set in Card-26, these have no meaning.
6) Flag IFIL in Card-32 is made 1. Filter collection efficiencies are given in Card-33, 34 or Card-33, 35.
7) Flag IGYA in Card-9 is made 1. Pressure of the automatically added nodes must be also set in Card-44.
8) Flag IFAOPT in Card-49 is made 1. Data of controlled valves are set in Card-50 and 51.
9) Flag IASTFG in Card-4 is made 0. Data for calculation of divided time steps are set in Card-5 and 6.

(3) CASE-3

1) Accident : explosion
2) Source term option : automatic calculation
3) Heat transfer calculation to wall: on
4) Aerosol transport calculation : off
5) Initial flow resistance option : user's input by branch data
6) Filter collection efficiency : default data

7) Automatic addition of check valve: off
8) Automatic open and shut of valve : off
9) Time step : divided time step

1),2) Flag PHENOM in Card-11 is made 2. Data for calculation of the source term, shapes of nodes and physical properties, are set in Card-15 and 16.
3) Flag ICALT in Card-11 is made 1. Data for calculation of heat transfer are set in Card-25 or Card-27 (for branch) and Card-38 or Card-42 (for node).
4) Flag ICALC in Card-17 is made 0.
5) Flag IDCAL in Card-10 is made 0. Initial flow resistances of respective branches are given in Card-26. In this case, Flag PINP in Card-43 must not be P.
6) Flag IFIL in Card-32 is made 0.
7) Flag IGYA in Card-9 is made 0.
8) Flag IFAOPT in Card-49 is made 0 .
9) Flag IASTFG in Card-4 is made 0.

5.2 Description of output

Calculational results for the following physical values can be obtained by TRANS-ACE. These results at the initial steady-state and calculational end time are stored for output automatically. Other output times are given in Card-7.

- Pressure at the nodes
- Gas temperature at the nodes
- Concentration of aerosol at the nodes
- Amount of deposited aerosol per unit time at the nodes
- Temperature of inner wall of the nodes
- Temperature of outside wall of the nodes
- Volume flow at the branches
- Deposition coefficients of aerosol per unit time at the ducts
- Amount of deposition of aerosol per unit time at the ducts
- Temperature of inner wall of the branches
- Temperature of outside wall of the branches
- Mass flow at the branches
- Summation of the amount of deposited aerosol at the branches
- Heat flux to inner wall of the nodes

·Heat flux from the outside wall of the nodes to the atmosphere
·Geometric average diameter and geometric standard deviation of aerosol before and after the filters
·Release rate of radioactive materials and activity concentration at the exit of the stack
·Decontamination factor at the exit of the stack

Time history of the following physical quantities can be obtained using a line-printer and plotter.
·Pressure at the nodes
·Flow resistance of the branches
·Temperature of gas at the nodes
·Temperature of the inner wall of the nodes
·Temperature of the outside wall of the the nodes
·Temperature of the inner wall of the ducts
·Temperature of the outside wall of the ducts
·Volume flow at the branches
·Mass flow at the branches
·Heat flux to the inner wall of the nodes
·Heat flux from the outside wall of the nodes to the atmosphere
·Heat flux to the inner wall of the branches
·Heat flux from the outside wall of the branches to the atomosphere
·Concentration of aerosol in the nodes
·Deposition rate of aerosol in the nodes
·Deposition rate of aerosol in the branches
·Deposition coefficients of aerosol in the nodes
·Deposition coefficients of aerosol in the branches
·Amount of collection of aerosol at the branches
·Radioactive concentration at the stack
·Radioactive release rate at the stack

6. SAMPLE CALCULATION

6.1 Accident scenario

Ventilation system for sample calculation is shown in Figure 2.4. It consists of 17 nodes (Boundary nodes: No. 1, No. 13 and No. 17; accident cell: No. 14) and 16 branches. Air supply duct system (Branch No. 1 to No. 7) is diluted by air from the dilution duct system (Branch No. 13 to No. 16). Initial volume flow rate of the air supply duct system, dilution duct system and filter system are 0.033 (m^3/s), 1.160 (m^3/s) and 1.2306 (m^3/s), respectively.

Solvent burns in the first model cell (Node No. 4). The solvent is 30 (%)TBP/n-dodecane solution of 0.03 (m^3). Burning area is 0.2304 (m^2) and depth of solvent is 0.48 (m). Ventilation flow to the accidental cell is 400 (m^3/hr). Conditions of boundary nodes and volume nodes are shown in Table 6.1 and Table 6.2, respectively. Physical properties of wall of accident cell are shown in Table 6.3. Branch data are shown in Table 6.4.

6.2 Function of TRANS-ACE usage

(1) Accident : solvent fire
(2) Source term setting : automatic calculation
(3) Heat transfer calculation to wall: on
(4) Aerosol transport calculation : on (default distribution)
(5) Initial flow resistance setting : automatic calculation
(6) Filter collection efficiency : user's input
(7) Automatic addition of check valve: off
(8) Automatic open and shut of valve : off
(9) Time step : divided time step (user's input)

Table 6.1 Boundary Node Data (Atmosphere : $1.01 \cdot 10^5$ (Pa))

Node number	Temperature (℃)	Pressure (PaG)
1	20.0	0.0
13	20.0	-98.0
17	20.0	0.0

Table 6.2 Volume Node Data

Node number	Temperature (℃)	Volume (m3)	Cross-sectional area (m^2)	Accident location
2	20.0	0.180	0.360	
3	20.0	0.471	0.362	
4	20.0	20.00	7.700	*
5	20.0	6.000	4.000	
6	20.0	0.132	0.018	
7	20.0	0.132	0.018	
8	20.0	2.820	0.282	
9	20.0	0.540	1.080	
10	20.0	0.540	1.080	
11	20.0	0.540	1.080	
12	20.0	2.820	0.282	
14	20.0	2.820	0.282	
15	20.0	5.640	0.282	
16	20.0	0.350	0.700	

Table 6.3 Wall Property of Accident Cell

Thickness (m)	Density (kg/m3)	Specific heat (J/kg·K)	Thermal conductivity (J/m·s·K)
0.218	968.0	575.6	4.0

Table 6.4 Branch Data

Branch No.	Component type	Initial flow resistance(PaG)	Cross-sectional area (m^2)	Maximum cross sectional area(m^2)	Length (m)
1	Filter	9.8	0.360	—	—
2	B-valve*	411.2	5.00***	0.0314	15.0
3	Duct	—**	0.0314	—	5.0
4	Duct	0.3	0.625	—	5.0
5	Duct	293.7	0.0176	—	5.0
6	Duct	280.0	0.0176	—	5.0
7	Duct	288.0	0.0176	—	5.0
8	Duct	2519.0	0.282	—	10.0
9	Filter	245.0	1.080	—	—
10	Filter	245.0	1.080	—	—
11	B-valve	1421.0	57.70***	1.080	—
12	Blower	-5684.0	0.282	—	—
13	Duct	1039.0	0.282	—	10.0
14	B-valve*	549.0	12.70***	0.2819	—
15	Duct	—**	0.282	—	20.0
16	Filter	157.0	0.700	—	—

* :Butterfly valve
** :Automatic calculation
***:Degree of open

6.3 Output list

6.3.1 Input data

```
*********************************************************************
*
*    TRANS-ACE  RUN DATA
*
*        REAL PROBLEM
*
*        1990.01.20
*
*********************************************************************
*              SIMULATION CONTROL DATA
*********************************************************************
*  TIMESTEP                    -------- DIV
*  RADIOACTIVITY INVENTORY     -------- USER
*  AEROSOL DISTORIBUTION       -------- LOG-NORMAL
*  FILTER EFFICIENCY           -------- USER
*  SOURCE TERM CALCULATION     -------- ON (FIRE)
*  INITIAL RESISTANCE-CALC     -------- ON
*  VALVE CONTROL               -------- ON
*  PREVENT BACK FLOW VALVE     -------- OFF
*************************************************  INPUTC  **********
*1. TITLE  CARD
 FIRE ACCIDENT IN CELL
*2. SIMULATION CONTROL CARD
* NOPT1
    0
*3. RUN CONTROL CARD
* RUNT    MAXIT    CONVRG     RBETA      FMIX MAXIT2   CONV2
   ST      1000     0.005       1.0             200    0.0005
*4. TIME STEP CARD (1)
*IASTFG    MAXV      MINV      MAXT      MINT
    0      2.00       0.1       0.1    0.0002
*5. TIME STEP CARD (2)
*  TSTCHG(1) TSTCHG(2) TSTCHG(3) TSTCHG(4) TSTCHG(5)
       0.0    5000.0
*6. TIME STEP CRAD (3)
*   TSTEP(1)  TSTEP(2)  TSTEP(3)  TSTEP(4)  TSTEP(5)
       5.0
*7. CALCULATION RESULTS OUTPUT TIME CONTROL CARD
* NSPOUT SOUT(1)   SOUT(2)   SOUT(3)   CHECK
    3    1000.0    2000.0    3000.0    6000.0
*8. CONSTITUTION OF THE VENTILATION SYSTEM INPUT CARD
*  N1   N2   N3   N4   N5 ISTACK
   16    3   14    1    4   13
*9. CHECK VALVE AUTOMATIC SETTTING CARD
* IGYA
    0
*10. FLOW RESISTANCE CALCULATION CONTROL CARD
* IDCAL
    1
*11. ACCIDENTAL CONDITION SETTING CARD
* PENM ICALT IBRM     HCELL
    1    1    4       2.2
*12. BURNING PARAMETERS INPUT CARD
*     GZAI       OXM       PSAI        EPS      GAMB2
      0.72       0.0       0.82      0.150        0.5
*13. SOLVENT FIRE CALCULATION DATA CARD (1)
*     QINL      DZPAN     BAREA       VTBP       VLSO
     400.0       0.48    0.2304       0.30       30.0
*14. SOLVENT FIRE CALCULATION DATA CARD (2)
```

```
*       CPD         PR       VMID        TSS       TAD
      0.246      0.673  0.257E-3      200.0 0.0
*15. EXPLOSION CALCULATION DATA CARD (1)
*       GRM NTYP
      10.00    1
*16. EXPLOSION CALCULATION DATA CARD (2)
*     SMOKEM     DMH2O      ROH2O      WRAD
       0.05     0.002        1.1     0.125
*17. AEROSOL DATA CARD (1)
*CALC
    1
*18. AEROSOL DATA CARD (2)
*     ALFNU         PK       ROUP         RG         DG       FALF      CDELT
        1.7       83.7    1.00E3        1.7    4.0E-7        0.9      0.005
*19. AEROSOL DATA CARD (3)
*IBUN  IBN
    0    1
*20. AEROSOL DATA CARD (4)
*     DI(1)      DI(2)      DI(3)
      5.E-7      5.E-6      5.E-5
*21. AEROSOL DATA CARD (5)
*   WTI(1)     WTI(2)     WTI(3)
 0.3333333 0.3333333 0.3333333
*22. RADIOACTIVE NUCLIDES DATA CARD (1)
*IFPDT LSTFL     CUO2       VWTR      RUGAS
    0   10     125.0       30.0        0.3
*23. RADIOACTIVE NUCLIDES DATA CARD (2)
*       RAD    RADCON        DIS         EF       NUCL
      0.153      19.1    1.0E-3     3.0E-3      SR-89
      0.102      12.7    1.0E-3     3.0E-3      SR-90
      0.096      12.0    1.0E-4        0.1     CS-137
     0.0584       7.3    1.0E-2        0.1     RU-103
      0.418      52.2    1.0E-2        0.1     RU-106
      0.418      52.2    1.0E-3        0.1     RH-106
      0.264      33.0       0.1        0.1      ZR-95
      0.557      69.6    1.0E-2        0.1      NB-95
      0.032       4.0    1.0E-3     5.0E-4     CE-141
      1.058     132.2    1.0E-3     5.0E-4     CE-144
      1.058     132.2    1.0E-5     5.0E-4     PR-144
    2.24E-4     0.028    2.7E-3        1.0       H-03
      0.102      12.7    1.0E-2     3.0E-3       Y-90
      0.222      27.8    1.0E-2     3.0E-3       Y-91
    1.12E-4     0.014    1.0E-4     3.0E-3     BA-140
    1.12E-4     0.014    1.0E-2     5.0E-4     LA-140
      0.362      45.2    1.0E-2     5.0E-4     PM-147
     4.1E-7   0.51E-4       4.0     5.0E-4       URAN
     6.4E-4      0.08       1.0     5.0E-4   PLUTONIUM
        0.0       0.0       0.0        0.0      DUMMY
*24. COMMON BRANCH DATA CARD (1)
* NOPT (1) - (6)
    3    1    4    3    4    3
*25. COMMON BRANCH DATA CARD (2)
*INITIAL VOLUME FLOW
*  IS   IE     VALUE
    1    7    0.0333
    8   12    1.2306
   13   16    1.1600
*DUCT TEMPERATURE
*  IS   IE     VALUE
    3   15      20.0
*DUCT ROU
```

```
*  IS   IE     VALUE
    3    3    7870.0
    4    4     968.0
    5    7    7750.0
    8   15    7870.0
*DUCT CP
*  IS   IE     VALUE
    3    3     460.0
    4    4     575.6
    5   15     460.0
*DUCT THICKNESS
*  IS   IE     VALUE
    3    3     0.005
    4    4     0.218
    5    7     0.005
    8   15      0.01
*DUCT THERMAL CONDUCTIVITY
*  IS   IE     VALUE
    2    3      25.5
    4    4      4.00
    5   15      25.5
*26.27.28. BRANCH DATA CARD (1) - (3)
    1    1    2    0.3600                F    2        9.8

    0    6    1
    2    2    3     32.13                BV          411.2                0.0314


    3    3    4    0.0314   15.0000      D             0.0
         3      90.0

    4    4    5     0.625    5.0000      D             0.3
        20      90.0

    5    5    6    0.0176    5.0000      D           293.7
         3       0.0

    6    6    7    0.0176    5.0000      D           280.0
         3      90.0
    7    7    8    0.0176    5.0000      D           288.0
         3       0.0

    8    8    9    0.2820   10.0000      D          2519.0
         5      90.0

    9    9   10    1.0800                F    2      245.0

    0    6    2
   10   10   11    1.0800                F    2      245.0

    0    6    2
   11   11   12      57.7                BV         1421.0                1.080


   12   12   13    0.2820                B    1    -5684.0

   13   14    8    0.2820   10.0000      D          1039.0
         5       0.0
                                                                          0.2819
   14   15   14      12.7                BV          549.0
```

```
   15   16   15    0.2820   20.0000    D            0.00
         5      90.0

   16   17   16    0.7000              F    2      157.0

    0    6    1
*29. BLOWER PROPERTY DATA (1)
*   J   NP
    1    5
*30. BLOWER PROPERTY DATA (2)
*       XB        FXB         XB        FXB         XB        FXB
       0.0     6400.0       0.75    6370.0       1.25    5880.0
 1.6666667    .5292.0 2.6666667        0.0
*31. FILTER FLOW RESISTANCE INPUT CARD
*   K        AKL        AKT
    1        0.0        0.0
    2    9.986E6       40.3
    3        0.0        0.0
    4        0.0        0.0
*32. FILTER COLLECTION EFFICIENCY INPUT CARD (1)
*IFIL
    0
*33. FILTER COLLECTION EFFICIENCY INPUT CARD (2)
*  DID2(1) - DID2(IBN)
  0.108E-6  0.120E-6  0.134E-6  0.150E-6  0.167E-6  0.186E-6
  0.209E-6  0.234E-6  0.261E-6  0.289E-6  0.326E-6
*34. FILTER COLLECTION EFFICIENCY INPUT CARD (3)
* ETID2(1) - ETID2(IBN)
      290.      280.      280.      290.      310.      400.
      500.      700.     1100.     1800.     3700.
*35. FILTER COLLECTION EFFICIENCY INPUT CARD (4)
* ETID3(1) - ETID3(IBN)
       2.9       2.8       2.8       2.9       3.1       4.0
       5.0       7.0      11.0      18.0      37.0
*36. BOUNDARY NODE DATA CARD
*BNNR        PB IBPFN       TB  IBTFN       CB IBCFN
    1              0              0              0
   13     -98.0    0              0              0
   17              0              0              0
*37. COMMON VOLUME NODE DATA CARD (1)
* NOPT (1) - (5)
    5    3    3    5    1
*38. COMMON VOLUME NODE DATA CARD (2)
*CELL THICKNESS
*  IS   IE     VALUE
    2    3     0.005
    4    4     0.218
    5    5     0.003
    6    7     0.005
    8   16      0.01
*CELL DENSITY
*  IS   IE     VALUE
    2    3    7870.0
    4    4     968.0
    5   16    7750.0
*CELL SPECIFIC HEAT
*  IS   IE     VALUE
    2    3     460.0
    4    4     575.6
    5   16     460.0
*CELL THERMAL CONDUCTIVITY
```

```
*  IS    IE      VALUE
    2     2       25.5
    3     3       25.2
    4     4        4.0
    5     7       25.5
    8    16       25.5
*CELL TEMPERATURE
*  IS    IE      VALUE
    2    16       20.0
*39. TIME FUNCTION CONTROL CARD
    1     0     0     1     1
*40.41.42. VOLUME NODE DATA CARD (1) - (3)
    2       0.18     0.3600

          3
    3      0.471     0.3620

          2
    4      20.0      7.7000     1     0     0     1     1

         20
    5       6.0      4.0000

          3
    6     0.132      0.0176
          2
    7     0.132      0.0176

          2
    8     2.820      0.2820

          2
    9      0.54      1.0800

          5
   10      0.54      1.0800

          5
   11      0.54      1.0800

          5
   12      2.82      0.2820

          2
   14      2.82      0.2820

         .2
   15      5.64      0.2820

          2
   16     0.350      0.7000

          5
*43. VOLUME NODE DATA CARD (4)
*PINP TINP CINP
   P     T
*44. NODE INITIAL PRESSURE DATA CARD
* P(1) - P(N2 + N3) (N2 AND N3 IN CARD-8)
              0.0      -9.8000000   -421.0000000   -490.0000000
   -490.3000000   -784.0000000    -1064.00000    -1352.00000
    -3871.00000    -4116.00000   -4361.000000   -5782.000000
           -98.0    -1137.00000   -588.0000000   -157.0000000
              0.0
```

```
*45. NODE INITIAL TEMPERATURE DATA CARD
* T(1) - T(N2 + N3)
          20.0          20.0          20.0          20.0
          20.0          20.0          20.0          20.0
          20.0          20.0          20.0          20.0
          20.0          20.0          20.0          20.0
          20.0
*46. NODE INITIAL AEROSOL DATA CARD
* C(1) - C(N2 + N3)
           0.0           0.0           0.0           0.0
           0.0           0.0           0.0           0.0
           0.0           0.0           0.0           0.0
           0.0           0.0           0.0           0.0
           0.0
*47.48. TIME FUNCTION INPUT DATA CARD (1) - (2)
* AEROSOL RELEASE RATE
    1    4    0
       0.0       0.0      1.65    0.6875       3.3       0.0
      20.0       0.0
* PRESSURE VARIATION
    0    2
       0.0       0.0      60.0       0.0
* TEMPERATURE VARIATION
    0    2
       0.0       0.0      60.0       0.0
* ENERGY RELEASE RATE
    1    4
       0.0       0.0      1.65   8.400E6       3.3       0.0
      20.0       0.0
* MASS RELEASE RATE
    1    4    0
       0.0       0.0      1.65      0.91       3.3       0.0
      20.0       0.0
*49. VALVE CONTROL CARD (1)
* OPT  VNO
    1    2
*50. VALVE CONTROL CARD (2)
*    IQBRA      QFIX          POPEN      QOPEN      INDZ
         2 0.1111111                      0.5
                              5.0E4                    15
*51. VALVE CONTROL CARD (3)
*   IFAVAL    FARATE          FAMIN      ISTOP     PSTOP
         2       5.0           30.0         -1
        14       5.0           30.0          1    -588.0
*52. CHECK VALVE AUTOMATIC ADDITION CONTROL CARD
*VLBR    BQOPEN   BFARATE   BFAMAX     BFAMIN
    1       5.0      30.0      5.0       30.0
   17       5.0      30.0      5.0       30.0
*53. CHECK VALVE AUTOMATIC ADDITION DATA CARD (1)
*WBND      DIFP        FA VLTP CRBR SLPD THETA
    1       0.0    0.2200    0    3    6
   17       0.0    0.2200    0    3    6
*54. CHECK VALVE AUTOMATIC ADDITION DATA CARD (2)
*WBND       VOL       RFA    DELSEL    RHOSEL    CPCELL    RPCELL    TCELLNCEL
    1      7.00      0.70      0.01    7750.0     460.0      25.5      20.0
   17      7.00      0.70      0.01    7750.0     460.0      25.5      20.0
*55. FLOW RESISTANCE AUTOMATIC CALCULATION DATA CARD (1)
* EVAL IVCT IDCT
    2    0    2
*56. FLOW RESISTANCE AUTOMATIC CALCULATION DATA CARD (2)
*IERVNO(1)-IERVNO(EVAL)
    2   14
```

```
*57. FLOW RESISTANCE OF VALVE AUTOMATIC CALCULATION DATA CARD
*VALV VLTP CRBR SLPD TETA
*58. FLOW RESISTANCE OF DUCT AUTOMATIC CALCULATION DATA CARD
*DUCT ILBO      RLBO        EPS'      DCAL
    3    1                1.5E-4
   15    1                1.5E-4
*59. CONDITION OF ATMOSPHERE
*    AMBBT      AMBCP      AMBKP      AMBRU      AMBMU      AMBTM      PZERO
   3.53E-3    1.00E3    2.49E-2      1.208    1.77E-5       20.0 1.01325E5
*60. PHYSICAL PROPERTIES OF FLUID DATA CARD (1)
* ANU       XKAPA       ROU        CP         EPSH        AMU       AIRM
   6.00E-3   5.08E-2     0.508    1.07E3    9.00E-2    3.66E-3    3.28E-5
*61. PHYSICAL PROPERTIES OF FLUID DATA CARD (2)
*    DINNU      VROOM       EMIT
    2.3E-5        3.0      0.550
*62. PLOT CONTROL DATA CARD (1)
    2    1    2    1    0    0    0    1    1    1
*63. PLOT CONTROL DATA CARD (2)
    0    0    0    2    0    0    0    1    1    1
*64. PLOT CONTROL DATA CARD (3)
*IPLOT ISCAL
    1    1
*65. PLOT CONTROL DATA CARD (4)
* PRESSURE
         4    1    3    4    5
         4    1    8    9   12
* PRESSURE DIFFERENCE
         2    9   10
* TEMPERATURE
         4    1    4    5    7
         4    1    8    9   10
* TEMP. OF NODAL INNER WALL
         4    4    5    9   11
* TEMP. OF NODAL OUTER WALL
*        4    4    5    9   11
* TEMP. OF DUCT INNER WALL
*        4    3    4    7    8
* TEMP. OF DUCT OUTER WALL
*        4    3    4    7    8
* VOLUME FLOW
         4    2    4    6   11
* MASS FLOW
         4    2    4    6   11
* HEAT FLOW TO INNER CELL WALL
         3    4    5    9
* HEAT FLOW FROM CELL WALL TO OUT
*        4    4    5    9   11
* HEAT FLOW TO INNER DUCT WALL
*        4    3    4    7    8
* HEAT FLOW FROM DUCT WALL TO OUT
*        4    3    4    7    8
* SMOKE CONCENTRATION
         3    4    7    9
         3    9   10   11
* DEPOSITION RATE IN CELL
*        2    4    5
* DEPOSITION RATE IN DUCT
*        2    4    5
* SMOKE DEPOSITION FACTOR
*        3    4    7    8
*        2    9   10
* ACCUMULATION OF SMOKE IN DUCTS & FILTERS
         2    9   10
```

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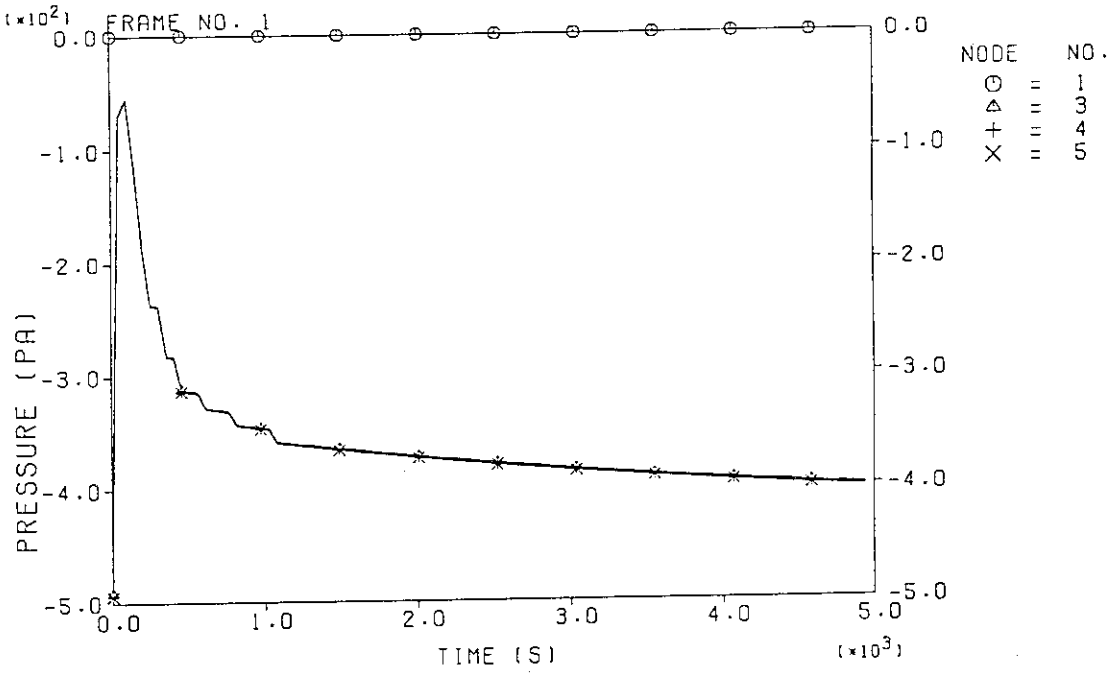
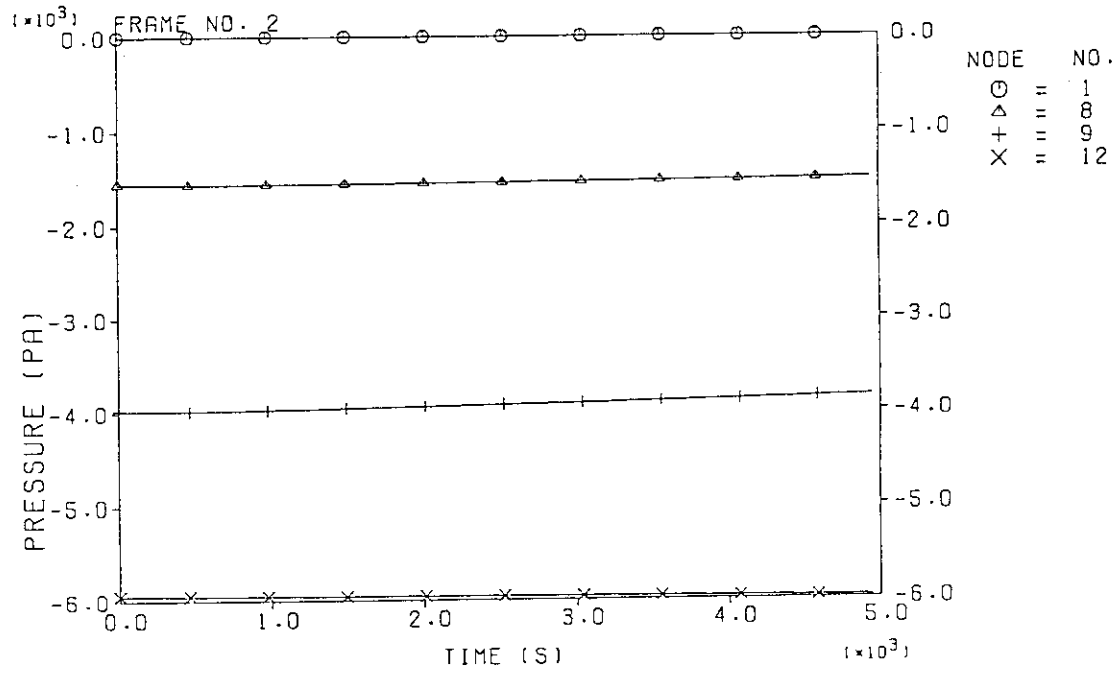
* RELEASE OF RADIOACTIVE MATERIALS TO ATMOSPHERE
* CONCENTRATION
LOG       1   13
* RELEASE RATE
LOG       1   13
```

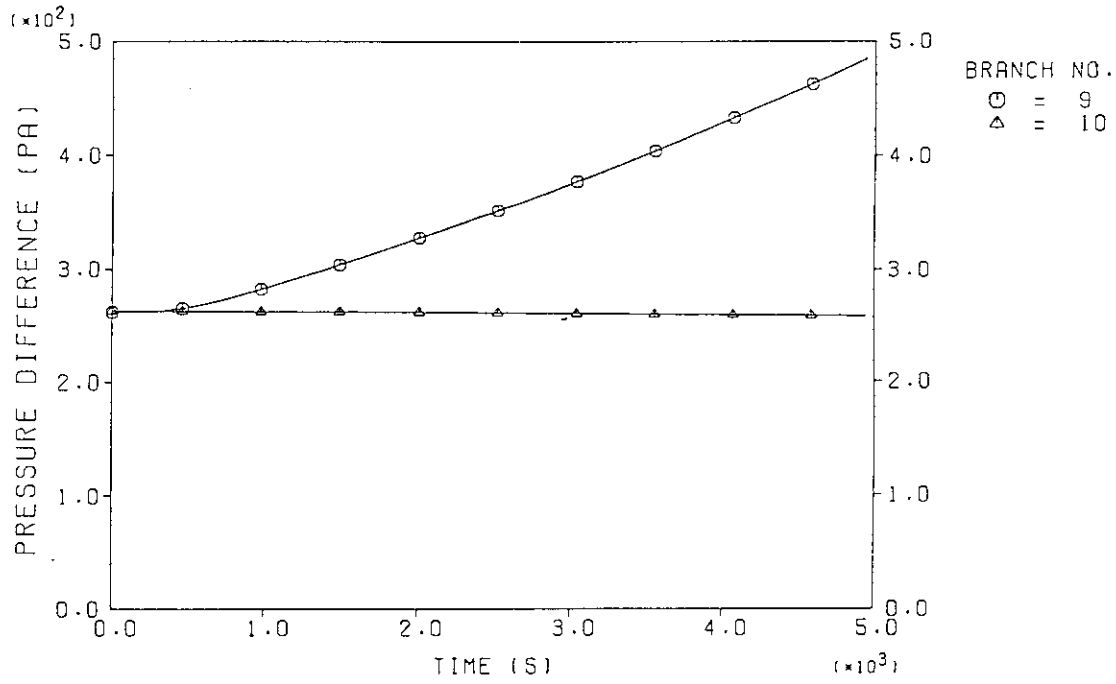
6.3.2 Calculation results

(1) Variation of pressure of nodes with the passage of time

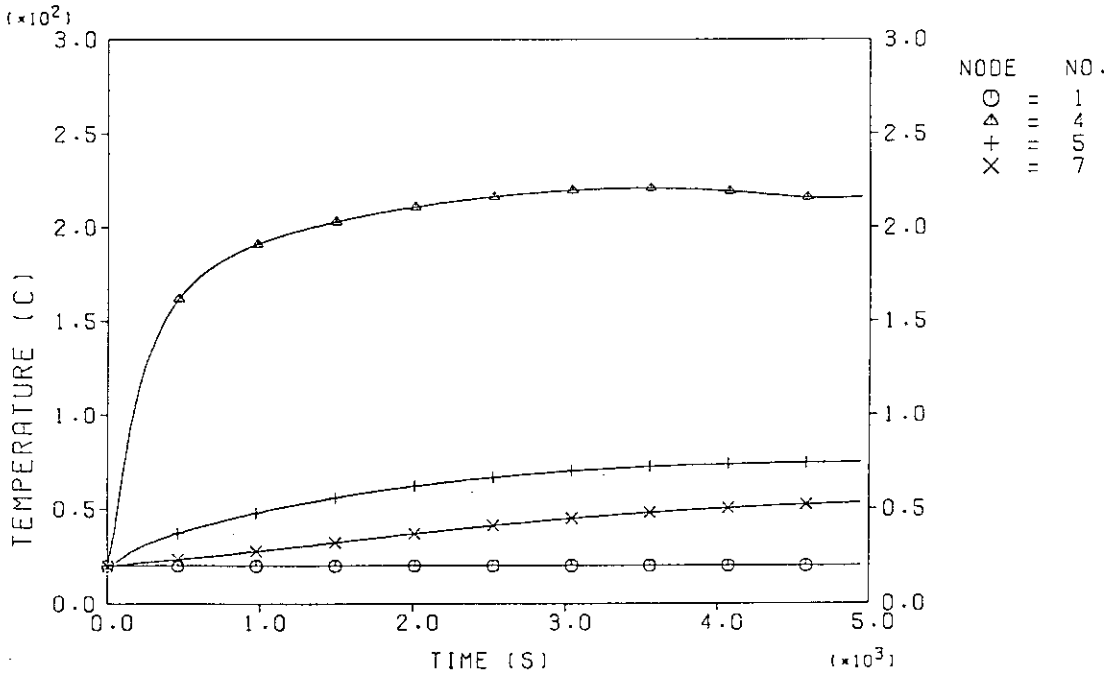


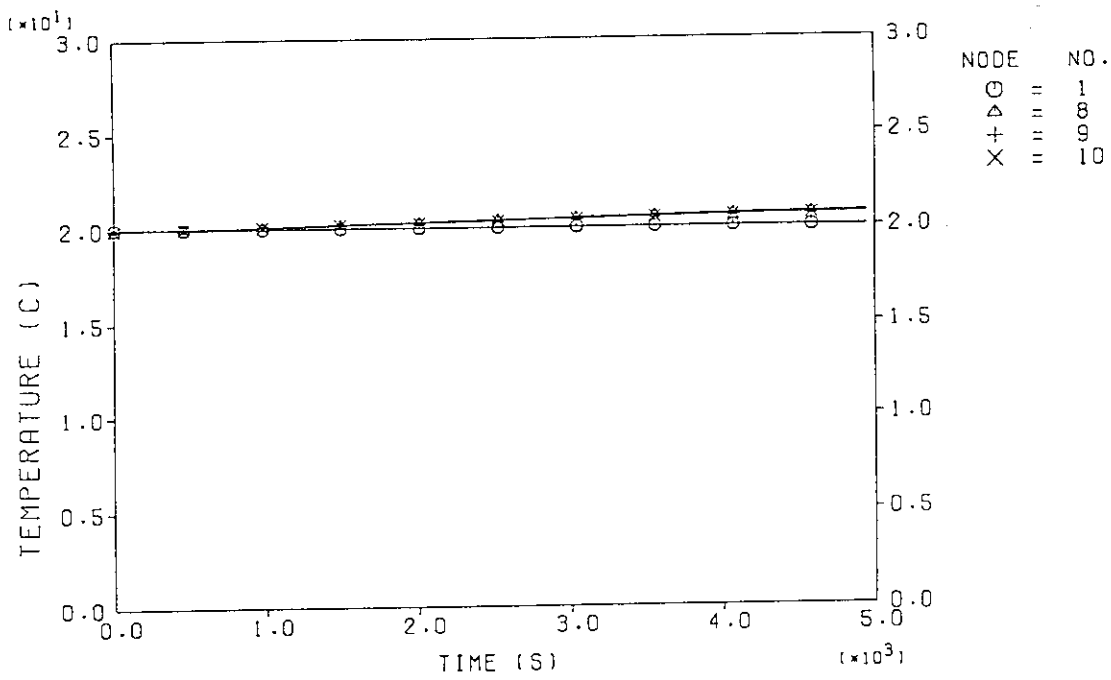


(2) Variation of pressure difference of branches with the passage of time

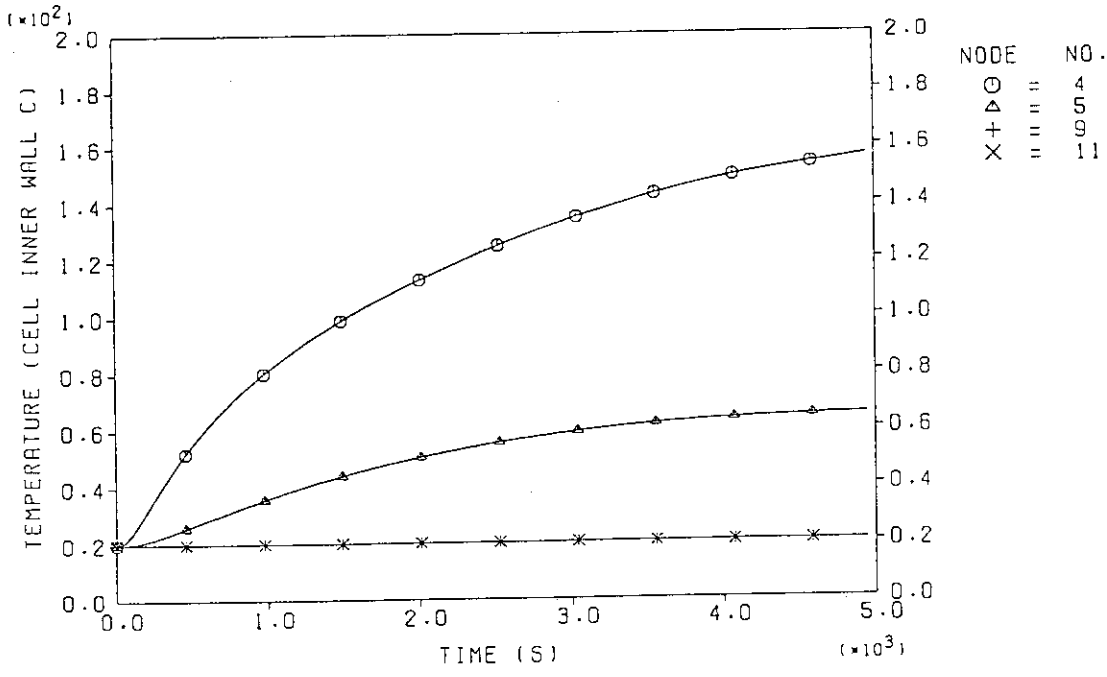


(3) Variation of temperature of nodes with the passage of time

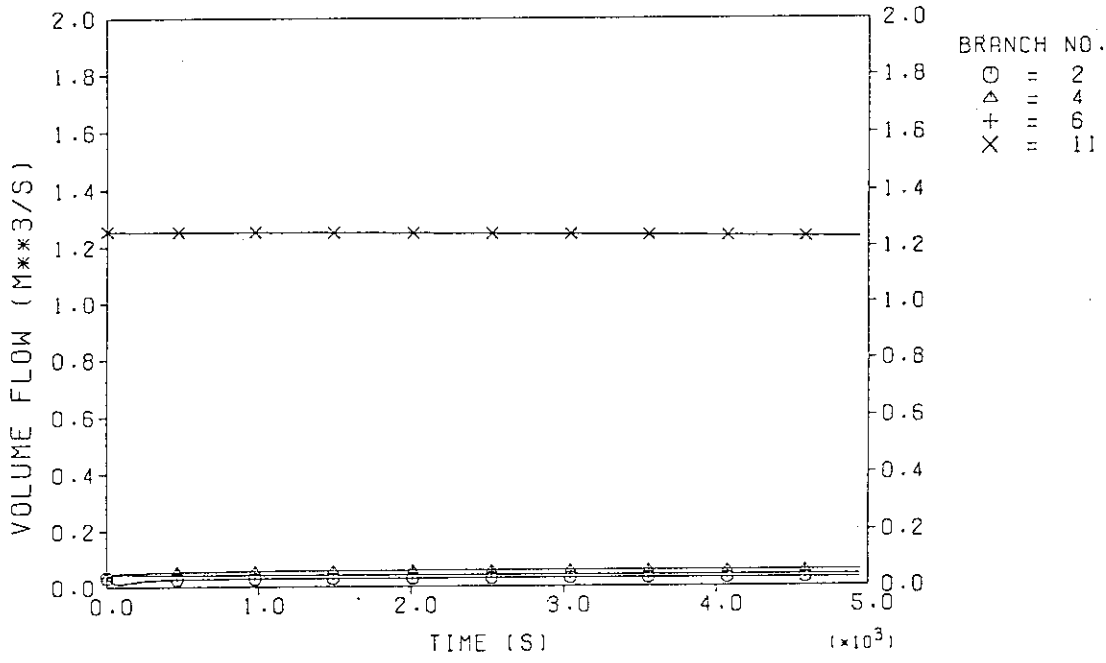




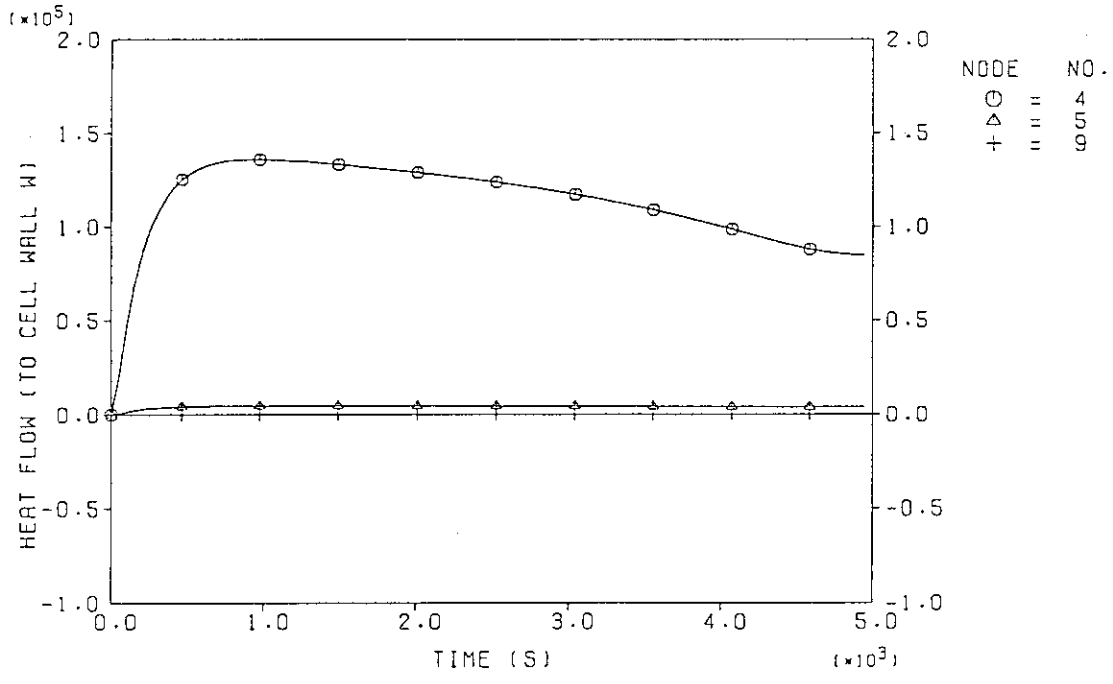
(4) Variation of temperature at inner wall of cell with the passage of time



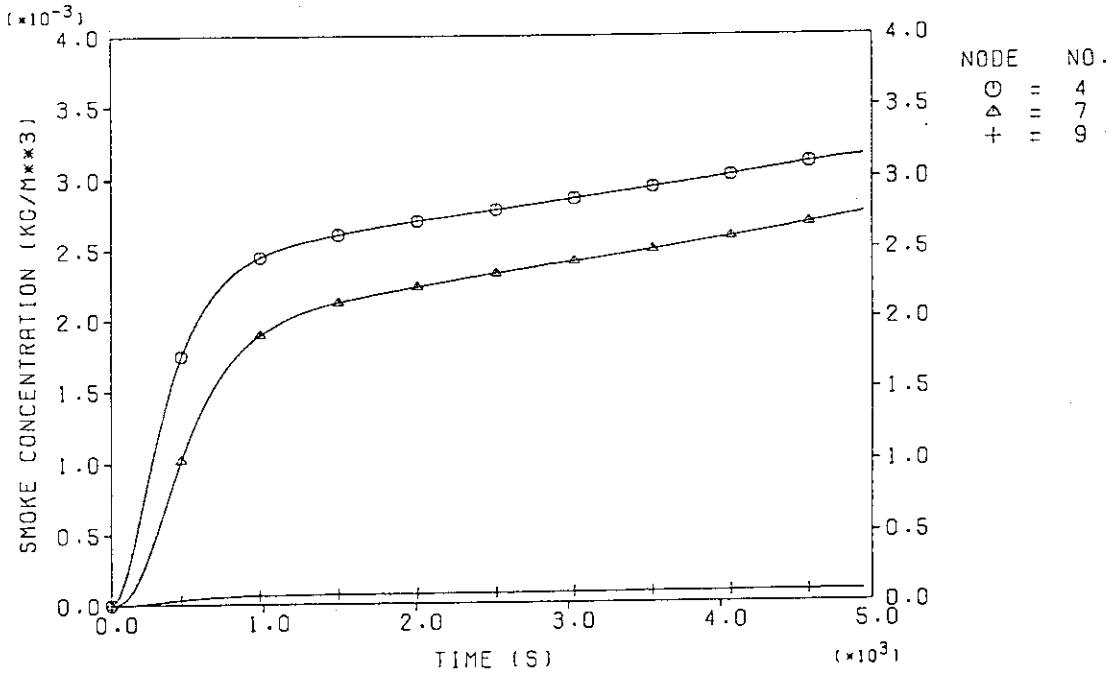
(5) Variation of volume flow rate of branches with the passage of time

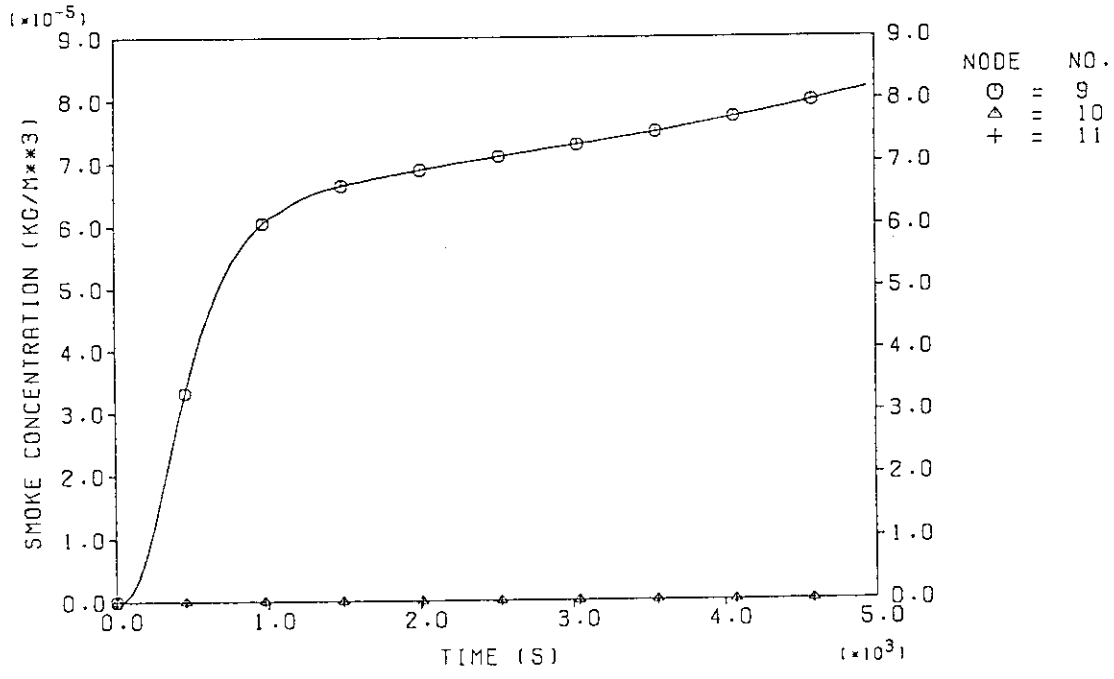


(6) Variation of heat flow to cell wall with the passage of time

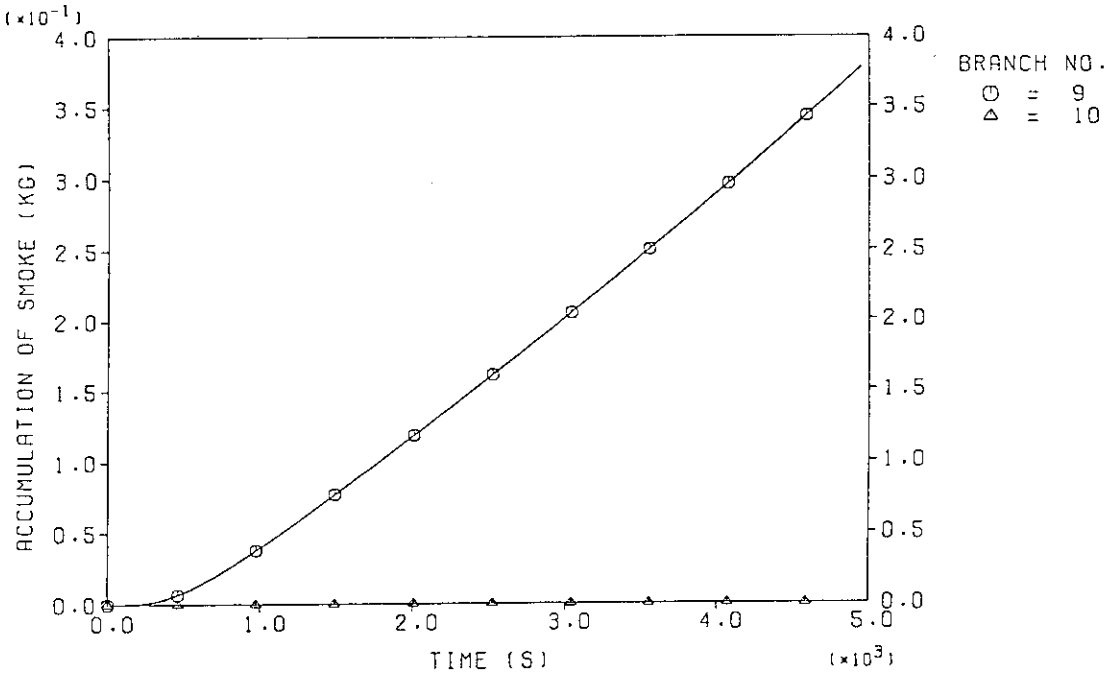


(7) Variation of smoke concentration of nodes with the passage of time

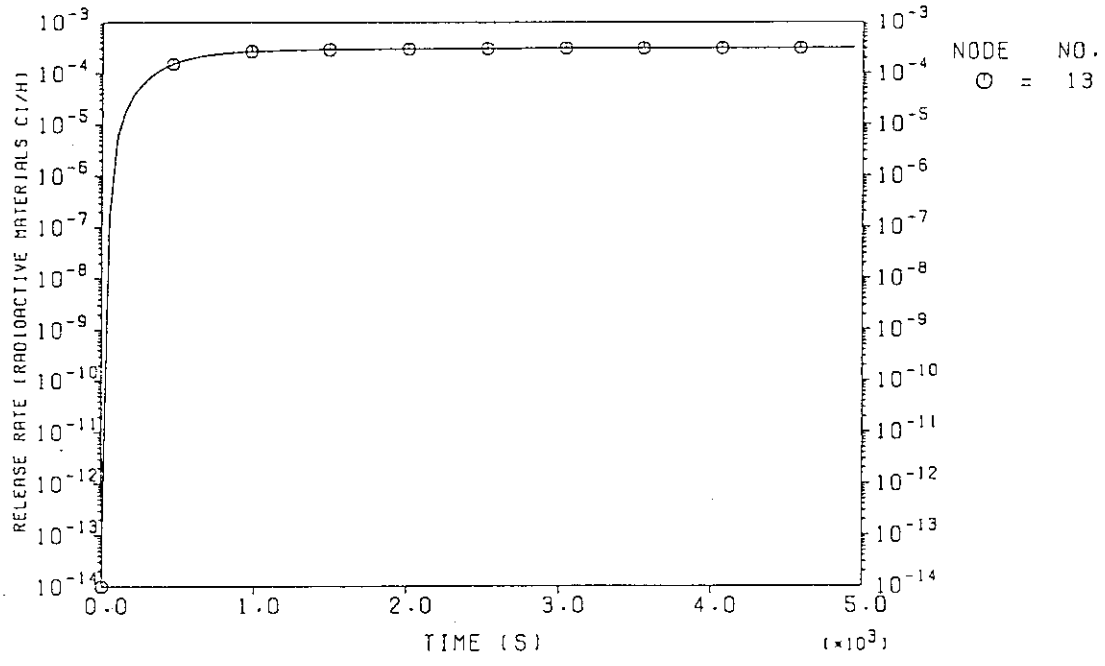




(8) Variation of accumulation of smoke in branches with the passage of time



(9) Variation of release rate of radioactive materials at stack with the passage of time



7. CONCLUSION

TRANS-ACE was developed for safety evaluation of nuclear fuel reprocessing plants. TRANS-ACE can calculate the synthetic accident analysis including the generation of accidental source term (solvent fire and explosion), transport and confinement of radioactive materials and heat transfer in the ventilation system of the facility and the final release of radioactive materials out of the facility by a combination of programmed functions.

TRANS-ACE is still not completed. Particularly, the auto-timestep setting function will have to be improved. To improve on TRANS-ACE, it will be necessary to collection data and bench-mark calculations based on some standard problems and a comparison with other accidental analysis codes. The defects of TRANS-ACE can be solved by carrying out bench calculations.

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Appendix-1 Particle size distribution of aerosol

Default particle size distribution of aerosol which is programmed in the code is shown in Table A.1.

Table A.1 Default Particle Size Distribution of Aerosol

i	D_i	$(W_T)_i$
1	$D_g\sigma_g^{-2.5}$	0.0122245
2	$D_g\sigma_g^{-2.0}$	0.0278347
3	$D_g\sigma_g^{-1.5}$	0.0655906
4	$D_g\sigma_g^{-1.0}$	0.1209776
5	$D_g\sigma_g^{-0.5}$	0.1746663
6	D_g	0.1974126
7	$D_g\sigma_g^{0.5}$	0.1746663
8	$D_g\sigma_g^{1.0}$	0.1209776
9	$D_g\sigma_g^{1.5}$	0.0655906
10	$D_g\sigma_g^{2.0}$	0.0278347
11	$D_g\sigma_g^{2.5}$	0.0122245

Appendix-2 Flow resistance of the HEPA filter

Relationship between volume flow and flow resistance of one-unit full-size HEPA filter (610 (mm)× 610 (mm)× 292 (mm)) is shown in Figure A.1. Relationship between volume flow and flow resistance of a full-size and half-size HEPA filter (610 (mm)× 305 (mm)× 292 (mm)) are shown in Table A.2. Flow resistances of the HEPA filter increase with increasing the volume flow increases and leaking occurs at 1000 (mmAq). Constants a and b in Eq.(3.3.24) which are calculated by use of the relationships are shown in Table A.3. K_L and K_T which are calculated by use of a and b, $\mu=1.95\times 10^{-5}$ (Pa·s), $\rho=1.0$ (kg/m^3) and A=0.186 (m^2) (half-size filter) or A=0.372 (m^2) (full-size filter) are shown in Table 4.4.

Table A.2 Relationship between Volume Flow and Flow Resistance of HEPA Filter

Flow resistance (Pa)	Volume flow (m^3/s)	
	Half-size	Full-size
245	0.2	0.4
523	0.417	0.833
1045	0.834	1.667
2730	1.667	3.333
5107	2.50	5.0
8410	3.33	6.667

Table A.3 Constants a and b in Eq. (4.4.23)

Filter size	a	b
Half-size	1042.9	581.6
Full-size	523.3	146.3

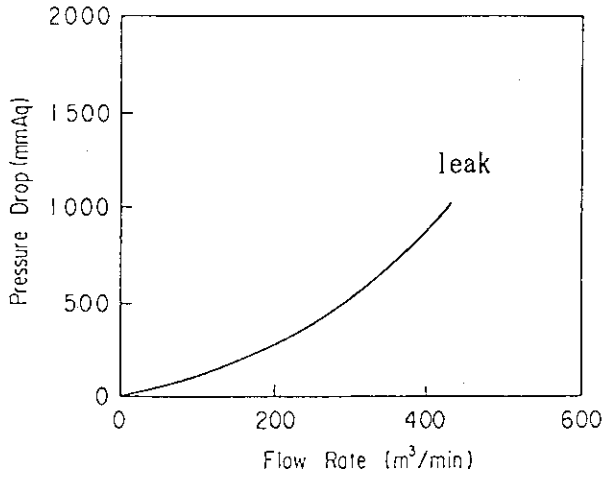

Fig. A.1 Relationship between volume flow and flow resistance of one-unit full-size HEPA filter.

Appendix-3 DF of the HEPA filter for collection of aerosol

Conservative empirical results between particle diameter of aerosol and DF (decontamination factor) are programmed as default data in TRANS-ACE. The empirical results are shown in Figure A.2.

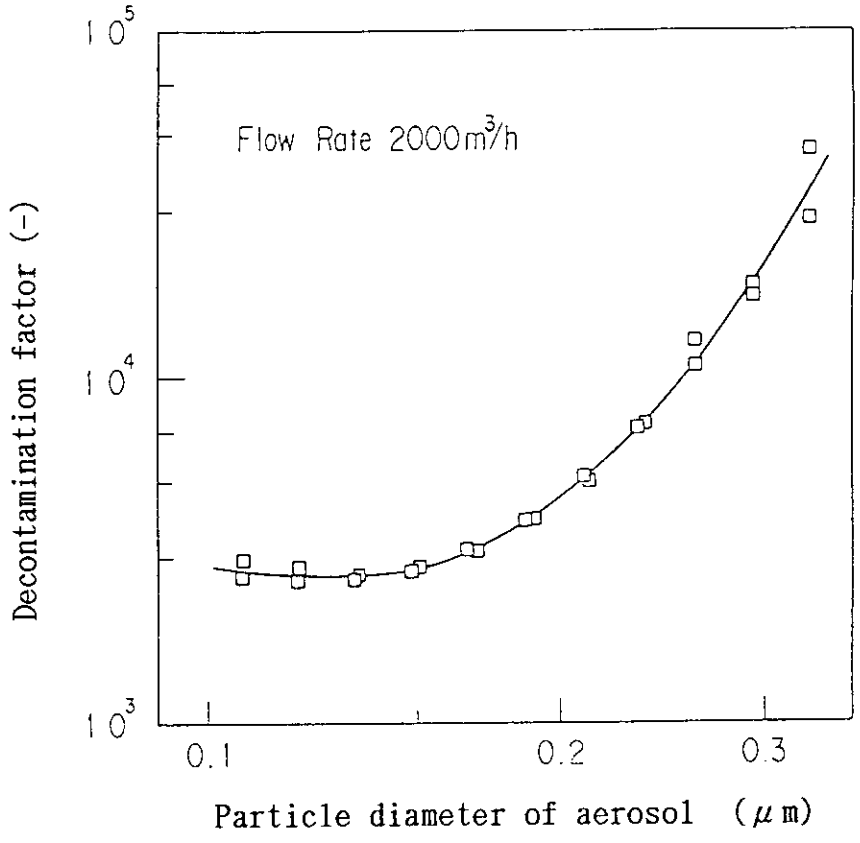

Fig. A.2 Empirical results between particle diameter of aerosol and DF.

Appendix-4 Increase of flow resistance of the HEPA filter with clogging

(1) Increase in flow resistance with smoke loading

Relationship between loaded smoke and flow resistance of a half-size HEPA filter is shown in Figure A.3. The relationship is shown by the following equation:

$$\Delta P_s(\mathrm{mmAq}) = 22.5753 + 0.2761L_s + 0.00065L_s^2$$

where L_s (g/one-unit filter) is the weight of collected smoke per one-unit filter.

(2) Increase in flow resistance with aerosol loading

Relationship between loaded aerosol (NaCl or JIS11-dust) and flow resistance of a full-size HEPA filter is shown by the following equations. The equations are obtained from severe filter condition experiments.

·NaCl

$$\Delta P_s(\mathrm{mmAq}) = 30.0 + 0.372L_s + 0.00135L_s^2$$

·JIS11-dust

$$\Delta P_s(\mathrm{mmAq}) = 28.9 + 0.0364L_s + 1.29\times 10^{-5}L_s^2$$

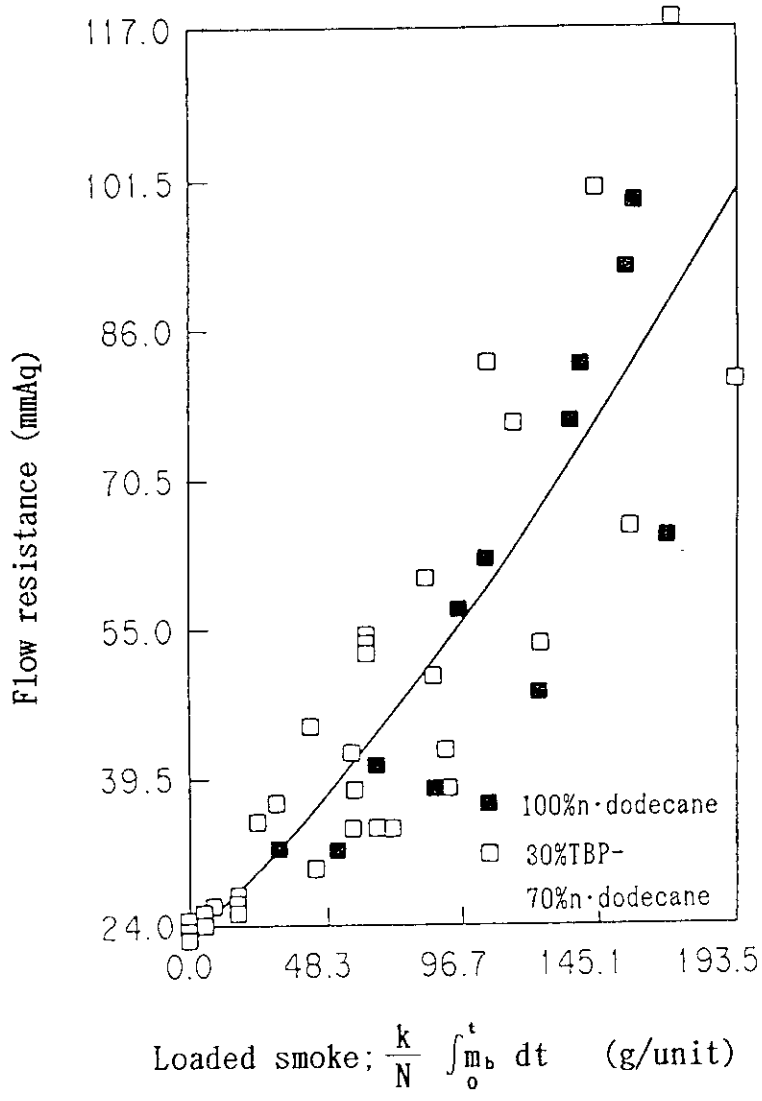

Fig. A.3 Relationship between loaded smoke and flow resistance of a half-size HEPA filter.