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FLOW NETWORK CALCULATION CODE FOR HEAT, MASS AND MOMENTUM TRANSFER IN A MULTICOMPONENT GAS MIXTURE FLOW WITH GRAPHITE CHEMICAL REACTIONS

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Japan Atomic Energy Research Institute

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Flow Network Calculation Code for Heat, Mass and Momentum Transfer in A Multicomponent Gas Mixture Flow with Graphite Chemical Reactions

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A flow network calculation code was developed to predict the thermo-hydraulic characteristics during a primary-cooling-pipe rupture accident in a high temperature gas cooled reactor such as the High Temperature Engineering Test Reactor (HTTR). The present calculation code deals with a natural convection of a multicomponent gas mixture (helium, nitrogen, oxygen, carbon monoxide and carbon dioxide) with graphite chemical reactions. One dimensional conservation equations of mass, momentum and energy for the gas mixture and equations of mass for gas species were solved by using a flow network model in the code. The calculation was performed for a flow channel system of an experimental apparatus simply simulating the cooling channels of the HTTR. The whole configuration of the flow channel is a reverse U shape, and the one vertical side of the reverse U shape consists of three parallel channels. Two of these channels are graphite ones. The entering flow rate, flow rates distributed to the parallel channels, generation volume of carbon monoxide and corrosion volume of the graphite could be calculated by the code.

Keywords: High Temperature Gas Cooled Reactor, Numerical Analysis, Flow Network Model, Reverse-U Shaped Flow Channel, Gas Mixture, Graphite Chemical Reactions, Pipe Rupture Accident

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* Institute of Nuclear Energy Technology, Tsinghua University

黒鉛の化学反応を伴う場合の多成分混合気体流れの熱・物質・流動管路網計算コード

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(1992年10月２日受理)

高温工学試験研究炉（ＨＴＴＲ）のような高温ガス炉における一次冷却系配管破断事故時の熱流動特性を予測するため、管路網計算コードを開発した。本計算コードでは、黒鉛の化学反応を伴う多成分混合気体（窒素、酸素、ヘリウム、一酸化炭素、二酸化炭素）の自然対流を扱う。一次元の混合気体の質量、運動量、エネルギー保存式と各成分気体の質量保存式を管路網モデルを用いて解いた。本計算では、ＨＴＴＲの冷却流路を簡単に模擬した実験装置の試験流路体系を対象とした。この試験流路は、全体には逆U字型をしており、この逆U字の一方の垂直流路部は、３並列流路となっている。３並列流路のうち２流路は黒鉛流路である。この数値解析コードによって、空気侵入流量、冷却流路配分流量、一酸化炭素の発生量、黒鉛腐食量を計算することができた。

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1. Introduction

Japan Atomic Energy Research Institute (JAERI) is building the High Temperature Engineering Test Reactor(1) (HTTR) at Oarai Research Establishment. The HTTR is a high temperature gas cooled reactor with thermal output of 30MW and outlet coolant temperature of 950°C, employing the pin-in-block type fuel, and has the capability to demonstrate nuclear process heat utilization using an intermediate heat exchanger.

A primary pipe rupture accident is one of the most critical (important) design-base accident of the HTTR. The accident starts from a guillotine break of the primary coaxial double pipe in the primary cooling system as shown in Fig. 1. When the primary pipe rupture takes place, a gas mixture containing oxygen enters the inside of the reactor vessel (RV) through the breach of the inner pipe from the reactor containment vessel (RCV), and the oxygen reacts with high temperature graphite. The graphite chemical reactions may cause corrosion of graphite, temperature rise and generation of inflammable gas; carbon monoxide. It has already been assured by extensive safety analysis and evaluation under the conservative assumption that no serious damages are caused to the reactor core and the RCV during and after the accident(2).

On the other hand, it is of great importance to know the real phenomena of the accident in order to understand the safety characteristics of the HTTR and in order to carry out a safety design with higher accuracy. In the analysis of the accident of the HTTR, the TAC-NC computer code was used to analyze the thermohydraulic characteristics and the GRACE computer code was used to analyze the graphite oxidation(3). Thus, the thermohydraulics and the graphite corrosion were separately calculated by using the TAC-NC code and GRACE code, respectively. The assumptions were considerably conservative in the analysis. For example, it was assumed that only the reaction; $C + \frac{1}{2} O_2 \rightarrow CO$ was taken into account as the chemical reaction of the graphite oxidation and no combustion of carbon monoxide was considered.

Accordingly, we developed a flow network calculation code to deal with heat, mass and momentum transfer with homogeneous (carbon monoxide combustion) and heterogeneous (graphite oxidation and Boudouard reaction) chemical reactions. The entering flow rate of the gas mixture, the corrosion volume of graphite and the generation volume of carbon monoxide were calculated in the code.

2. Nomenclature

- A : Coefficient of Eq.(3.15)
- B : Coefficient of Eq.(3.15)
- c_p : Specific heat at constant pressure
- Da : Damköhler number
- d_k : Tube diameter of k th branch
- d_0 : Tube diameter of reference branch
- f : Friction factor
- f : Generation ratio of carbon monoxide mole fraction to carbon dioxide one
- G : Flow rate (=ρU)
- g : Gravitational acceleration (=9.807)
- k^+ : Chemical reaction rate constant
- M : Molecular weight
- m : Solid/gas chemical reaction rate (=mass flux)
- Nu : Nusselt number
- P : Dimensionless pressure
- p : Pressure
- Pr : Prandtl number
- Q : Generation heat due to carbon monoxide combustion
- R : Gas/gas chemical reaction rate
- Re : Reynolds number
- R_g : Gas constant (=8.314)
- Sc : Schmidt number
- Sh : Sherwood number
- T : Temperature
- T_K : Absolute temperature
- t : Time
- U : Dimensionless velocity
- u : Velocity
- ΔV : Volume of node
- X : Dimensionless axial distance
- x : Axial distance
- Δx : Length of branch

Suffix

b : Bulk

C : Graphite

i : Gas species

j : The number of the node

k : The number of the branch

n : The number of the time step

w : Wall

0 : Reference (Inlet or Atmosphere)

Greeks

α : Heat transfer coefficient

β : Mass transfer coefficient

ε_k : $=d_k/d_0$

η : Pressure loss coefficient

Θ : Dimensionless temperature

θ : Angle of branch from gravitational direction

λ : Thermal conductivity

ρ : Density

τ : Dimensionless time

ν : Kinematic viscosity

ω : Mass fraction

Here, all units used are the International System of Units (SI units).

3. Numerical Analysis

3.1 Basic Equation

One-dimensional transient equations of mass, momentum and energy conservation for a gas mixture are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = S_k m_c, \tag{3.1}$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial p}{\partial x} - \left(\frac{4}{d_k} f + \frac{1}{\Delta x}\sum_{\ell}\eta_{\ell}\right)\frac{\rho |u|}{2} u + \rho g \cos\theta_k, \tag{3.2}$$

$$\rho \frac{\partial}{\partial t}(c_p T) + u \frac{\partial}{\partial x}(c_p T) = S_k \alpha (T_w - T) + Q, \tag{3.3}$$

Suffix

- b : Bulk
- C : Graphite
- i : Gas species
- j : The number of the node
- k : The number of the branch
- n : The number of the time step
- w : Wall
- 0 : Reference (Inlet or Atmosphere)

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$$\rho \frac{\partial}{\partial t}(c_p T) + u \frac{\partial}{\partial x}(c_p T) = S_k \alpha (T_w - T) + Q, \tag{3.3}$$

here, k represents the number of the branch.

$$S_k = \frac{\pi\ d_k}{\frac{\pi}{4}\ d_k^2} = \frac{4}{d_k} . \tag{3.4}$$

Ideal gas is assumed. The density of the gas mixture is given as:

$$\rho = \frac{pM}{R_g\ T_k} . \tag{3.5}$$

A one-dimensional transient equation of mass conservation for each gas species is in the following;

$$\rho \frac{\partial \omega_i}{\partial t} + \rho u \frac{\partial \omega_i}{\partial x} = S_k\ \rho \beta_i (\omega_{w_i} - \omega_i) + R_i . \tag{3.6}$$

The gas mixture in the accident may consist of five gas species; helium, oxygen, carbon monoxide, carbon dioxide and nitrogen. In the above equations, i=1, 2, 3, 4 and 5 show helium, oxygen, carbon monoxide, carbon dioxide and nitrogen, respectively.

We convert above equations to dimensionless ones by the following normalization:

$$\left. \begin{aligned} X &= \frac{x}{d_0}, \\ \varepsilon_k &= \frac{d_k}{d_0} , \\ \Delta X &= \frac{\Delta x_k}{d_k} . \end{aligned} \right\} \tag{3.7}$$

$$\left. \begin{aligned} U &= \frac{u}{u_0} . \ (u_0 = \sqrt{\frac{\Delta\rho\ g\ d_0}{\rho_0}},\ \Delta\rho = \rho_0 - \rho_{min}) \\ G &= \rho^* U , \\ P &= \frac{p'}{\rho_0\ u_0^2} ,\ (p' = p - p_0,\ \frac{\partial p_0}{\partial x} = \rho_0 g\ \cos\theta_k) \\ \Theta &= \frac{T}{T_{max}} , \\ \tau &= \frac{t}{\frac{d_0}{u_0}} . \end{aligned} \right\} \tag{3.8}$$

$$\left.\begin{aligned}
&Da_{w_C} = \frac{4m_C}{\rho_0\ u_0}\ \frac{1}{\varepsilon_k}\ , && Sh_i = \frac{\beta_i\ d_0}{D_{He/i}}\ , \\
&Da_i = \frac{d_0\ Ri}{\rho_0\ u_0}\ , && Q^* = \frac{d_0\ Q}{\rho_0\ u_0\ c_{p0}\ T_{max}}\ , \\
&Re = \frac{d_0\ u_0}{\nu_0}\ , && \Delta\rho_k^* = -\frac{\rho_0 - \rho}{\rho_0 - \rho_{min}} \cos\theta_k\ , \\
&Pr = \frac{\rho_0\ c_{p0}\ \nu_0}{\lambda_0}\ , && \rho^* = \frac{\rho}{\rho_0}\ , \\
&Sc_i = \frac{\nu_0}{D_{He/i}}\ , && c_p^* = \frac{c_p}{c_{p0}}\ . \\
&Nu = \frac{\alpha\ d_0}{\lambda_0}\ , &&
\end{aligned}\right\} \qquad (3.9)$$

The above normalization derives dimensionless equations from Eqs.(3.1)-(3.3), and (3.6);

$$\frac{\partial\rho^*}{\partial\tau} + \frac{\partial}{\partial X}(\rho^* U) = Da_{w_C} \qquad (3.10)$$

$$\rho^* \frac{\partial U}{\partial\tau} + \rho^* U \frac{\partial U}{\partial X} = -\frac{\partial P}{\partial X} - \left(4f + \frac{d_k}{\Delta x_k}\sum_{\ell}\eta_{\ell}\right)\frac{\rho^*|U|}{2\ \varepsilon_k} U + \Delta\rho_k^* \qquad (3.11)$$

$$\rho^* \frac{\partial}{\partial\tau}(c_p^*\ \Theta) + \rho^* U \frac{\partial}{\partial X}(c_p^*\ \Theta) = \frac{4}{\varepsilon_k}\ \frac{Nu}{Re\ Pr}(\Theta_w - \Theta) + Q^* \qquad (3.12)$$

$$\rho^* \frac{\partial\omega_i}{\partial\tau} + \rho^* U \frac{\partial\omega_i}{\partial X} = \frac{4}{\varepsilon_k}\ \frac{Sh_i}{Re\ Sc_i}\ \rho^*(\omega_{w_i} - \omega_i) + Da_i \quad (i = 1 \sim 5) \qquad (3.13)$$

3.2 Flow Network Model

We can solve the differential equations of Eqs.(3.10)-(3.13) by using the finite difference method. However, much memory capacity and calculation time are necessary when the calculation is executed for the cooling channel system of the HTTR because of many cooling channels. Therefore a one-dimensional flow network model is applied to the problem. One cooling channel can be expressed by using a branch and the branch is connected to other branches at node in the flow network model. No distributions of variables are considered in the node, that is, the node is assumed as a point without volume. Thus, we can easily describe the complicated cooling channel system with these branches and nodes.

In the branch, we can obtain basic equations of momentum and energy conservation for the gas mixture and of mass conservation for each gas species by integrating Eqs.(3.11) to (3.13) from the inlet of the branch to the outlet in the X axis direction.

$$G_{x+\Delta x} - G_x = Da_{w_C}\ \Delta X + \{(\rho^*)^n - (\rho^*)^{n+1}\}\ \frac{\Delta X}{\Delta\tau} \tag{3.14}$$

$$\left.\begin{aligned} &P_x - P_{x+\Delta x} = A_k\ G_k + B_k \\ &\quad A_k = (4\ \Delta Xf + \sum_{\ell} \eta_\ell)\ \frac{|G_k|}{2\ \varepsilon_k\ \rho^*} + \frac{\Delta X}{\Delta\tau} \\ &\quad B_k = (\frac{G^2_{x+\Delta x}}{\rho^*_{x+\Delta x}} - \frac{{G_x}^2}{{\rho^*}_x}) + (\Delta{\rho^*}_k - \frac{G_k}{\Delta\tau})\Delta X \end{aligned}\right\} \tag{3.15}$$

$$\begin{aligned} &\{({c_p}^*\ \Theta)_{x+\Delta x} - ({c_p}^*\ \Theta)_x\}G_k \\ &\quad = \{\frac{4\ Nu}{\varepsilon_k\ Re\ Pr}(\Theta_w - \bar{\Theta}) + Q^*\}\Delta X \\ &\qquad + \{({c_p}^*\ \Theta)^n - (c_p\ \Theta)^{n+1}\}\ \frac{\rho^*\ \Delta X}{\Delta\tau} \end{aligned} \tag{3.16}$$

$$\begin{aligned} &\{(\omega_i)_{x+\Delta x} - (\omega_i)_x\}G_k \\ &\quad = \{\frac{4\ Sh_i\ \rho^*}{\varepsilon_k\ Re\ Sc_i}(\omega_{w_i} - \bar{\omega}_i) + Da_i\}\Delta X \\ &\qquad + \{(\omega_i)^n - (\omega_i)^{n+1}\}\ \frac{\rho^*\ \Delta X}{\Delta\tau} \end{aligned} \tag{3.17}$$

If no chemical reaction takes place in the branch, Damköhler number in Eq.(3.14) is equal to zero. In the node, basic equations of mass and energy conservations for the gas mixture and of mass conservation for each gas species are expressed in the following.

$$\Sigma(d^2\ G)_k = \Sigma(Da_{w_C}\ \Delta X\ d^2)_k, \tag{3.18}$$

$$\Sigma(G\ {c_p}^*\ \Theta)_k = 0 \tag{3.19}$$

$$\Sigma(G\ \omega_i)_k = 0 \tag{3.20}$$

Here, in Eq.(3.18), the gas flow rate entering the node is defined to be positive and the flow rate going out of the node to be negative. The signs of the heat flow rate of $(G{c_p}^*\ \Theta)$ in Eq.(3.19) and the mass flow rate of (Gω) in Eq.(3.20) are decided in the similar way as the flow rate. The node temperature and the node mass fraction are used as inlet values of the branch for the outflow from the node and the temperature and mass fraction of the branch outlet are used to calculate the node values.

An experimental apparatus has been manufactured to simulate the natural convection simply during the primary pipe rupture accident in the HTTR. The flow channel of the experimental apparatus is a reverse U shaped circular tube. The one side of the reverse U tube is a hot region and the other is a cold region as shown in Fig. 2. The cold and hot regions simulate the inlet cooling annular channel around the reactor core and the cooling channels in the reactor core, respectively. The hot region of the reverse U tube consists of three parallel vertical channels. One of the three channels is a cold channel and the rest are hot channels. The hot channel is a graphite circular tube placed in an electric furnace which is represented as Test section A or C as shown in Fig. 2. The temperature difference between the three channels simulates the one in the radial direction of the reactor core. Figure 3 shows the flow network used here for modeling the experimental apparatus. No.5 and 11 branches in Fig. 3 are graphite channels. The arrows in Fig. 3 denote the positive direction of the flow rate. The dimensions of the branches in Fig. 3 are shown in Table 3.

3.3 Algebraic Equation

In the present flow network shown in Fig. 3, the right-hand term in Eq.(3.21) is necessary only when the node connects to the No.5 or No.11 branch. The other nodes do not require the right-hand term in Eq.(3.21).

$$\Sigma(d^2G)_k = (Da_{w_C}\ \Delta X\ d)_{k'} \quad (k' = 5 \text{ or } 11) \tag{3.21}$$

Here, the sign of G_k is defined as plus for the direction of the arrows shown in Fig. 3. For the pressure, in the closed circuit of the flow network model, the following equation is obtained from Eq.(3.15):

$$\Sigma(A_k\ G_k) = -\ \Sigma B_k \tag{3.22}$$

In the present calculation three closed circuits are chosen from the flow network in Fig. 3:

(1) No.1 closed circuit: 2-3-4-5-6-7-13-12-11-10-9-8

(2) No.2 closed circuit: 8-9-10-11-12-13-19-18-17-16-15-14

(3) No.3 closed circuit: 1-14-15-16-17-18-19-20-21-22-23-24-25-26-27

(These figures denote the branch numbers in Fig. 3.)

The energy equations of the gas mixture at the branch and the node are written as follows:

$$G_k(c_p{}^* \Theta)_{x+\Delta x} - G_k\{(c_p{}^* \Theta)_{x_i} \delta_k^+ + (c_p{}^* \Theta)_{x_{i+1}} \delta_k^-\} \tag{3.23}$$

$$= \{\frac{4\ Nu}{\varepsilon_k\ Re\ Pr} (\Theta_w - \bar{\Theta}) + Q^*\}\Delta X$$

$$+ \{(c_p{}^* \Theta)^n - (c_p{}^* \Theta)^{n+1}\} \frac{\rho^* \Delta X}{\Delta\tau}$$

$$(c_p{}^* \Theta)_{x_i}\ \Sigma(G_k\ \delta_k^+) - \Sigma\{(c_p{}^* \Theta)_{x+\Delta x_k}\ G_k\ \delta_k^-\} = 0 \tag{3.24}$$

$$\delta_k^+ = \max(\frac{G_k}{|G_k|}\ ,\ 0),\quad \delta_k^- = \max(\frac{-G_k}{|G_k|}\ ,\ 0) \tag{3.25}$$

respectively. In Eq.(3.23) the i th or (i+1) th node in the k th branch is selected as the node of inlet side, judging from the flow direction in the k th branch. In the energy equation at the i th node, k (k = 1,2,3,•••) branches connect to the i th node as shown in Fig. 4. In Eq.(3.24), $(c_p{}^* \Theta)_{x+\Delta x}$ is the outlet value of the k th branch and $(c_p{}^* \Theta)_{x_i}$ is the node value of the i th node. In Eq.(3.25), max(X1,X2) denotes the followings;

if X1 > X2, then max(X1,X2) = X1

if X1 < X2, then max(X1,X2) = X2.

The equations of the mass conservation for each gas species at the branch and the node can be expressed in the same manner as the energy equations.

$$G_k(\omega_i)_{x+\Delta x} - G_k\{(\omega_i)_{x_i}\ \delta_k^+ + (\omega_i)_{x_{i+1}}\ \delta_k^-\} \tag{3.26}$$

$$= \{\frac{4\ Sh_i\ \rho^*}{\varepsilon_k\ Re\ Sc_i}(\omega_{w_i} - \bar{\omega}_i) + Da_i\}$$

$$+ \{(\omega_i)^n - (\omega_i)^{n+1}\}\frac{\rho^*\ \Delta X}{\Delta\tau}$$

$$(\omega_i)_{x_i}\ \Sigma(G_k\ \delta_k^+) - \Sigma\{(\omega_i)_{x+\Delta x_k}\ G_k\ \delta_k^-\} = 0 \tag{3.27}$$

In the above equations of Eqs.(3.21) to (3.27), unknown values are in the following:

(a) Mass flow rate of gas mixture in the k th branch ; G_k

(b) Outlet temperature of gas mixture in the k th branch ; $T_{0,k}$

(c) Outlet mass fraction of each gas species in the k th branch ; $\omega_{0,k}$

(d) Temperature of gas mixture at the i th node ; $T_{N,i}$

(e) Mass fraction of each gas species at the i th node ; $\omega_{N,i}$

Three simultaneous linear equations for the mass flow rate, temperature and mass fraction are obtained from Eqs.(3.21) to (3.27) by assuming that factors like A_k in Eq.(3.22) are tentatively constant, although those factors are functions of the flow rate, temperature or mass fraction. First, the flow rate is solved by an iteration procedure, then the temperature of the gas mixture and the mass fraction of each gas species are solved. Figure 5 shows the flow chart of the code. The calculation at the certain time step is repeated until the converging conditions are satisfied, then it goes ahead to the next time step.

The present computer program is shown in Appendix.

3.4 Correlations of Heat and Mass Transfers and Pressure Loss

Friction factor, heat transfer and mass transfer coefficients are given by the following equations(4):

$$f_{x_1-x_2} = \frac{x_2\ f_{app}(x_2) - x_1\ f_{app}(x_1)}{x_2 - x_1} \tag{3.28}$$

$$\Delta\rho \equiv \frac{4(x_2 - x_1)}{d}\ f_{x_1-x_2}\ \frac{\rho u^2}{2} \tag{3.29}$$

$$f_{app}(x)\mathrm{Re} = \frac{3.44}{\sqrt{x^+}} + \frac{1.25/(4x^+) + 16 - 3.44/\sqrt{x^*}}{1 + 2.1 \times 10^{-4}(x^+)^{-2}} \tag{3.30}$$

$$\Delta p_{0-x} \equiv \frac{4x}{d}\ f_{app}(x)\frac{\rho u^2}{2} \tag{3.31}$$

$$\alpha_{x_1-x_2} = \frac{x_2 \Delta T_{0-x_2} \lambda_{0-x_2} Nu_{0-x_2} - x_1 \Delta T_{0-x_1} \lambda_{0-x_1} Nu_{0-x_1}}{d(x_2 - x_1)\Delta T_{x_1-x_2}} \tag{3.32}$$

$$Nu_{0-x} = \left.\begin{array}{ll} 1.615(x^*)^{-\frac{1}{3}} - 0.7, & x^* \le 0.005 \\ 1.615(x^*)^{-\frac{1}{3}} - 0.2, & 0.005 < x^* < 0.03 \\ 3.657 + 0.0499(x^*)^{-1}, & x \ge 0.03 \end{array}\right\} \tag{3.33}$$

$$x^* = \frac{\frac{x}{d}}{Re\ Pr} \tag{3.34}$$

$$\Delta T_{x_1-x_2} = \frac{T_{b_{x_2}} - T_{b_{x_1}}}{\ell n \dfrac{T_w - T_{b_{x_1}}}{T_w - T_{b_{x_2}}}} \tag{3.35}$$

$$\beta_{x_1-x_2} = \frac{x_2\ \beta_{0-x_2}\ \Delta\omega_{0-x_2} - x_1\ \beta_{0-x_1}\ \Delta\omega_{0-x_1}}{(x_2 - x_1)\Delta\omega_{x_1-x_2}} \tag{3.36}$$

$$Sh_{0-x} = \left.\begin{array}{ll} 1.615(x^{**})^{-\frac{1}{3}} - 0.7, & x^{**} \le 0.005 \\ 1.615(x^{**})^{-\frac{1}{3}} - 0.2, & 0.005 < x^{**} < 0.03 \\ 3.657 + 0.0499(x^*)^{-1}, & x \ge 0.03 \end{array}\right\} \tag{3.37}$$

$$x^{**} = \frac{\frac{x}{d}}{Re\ Sc_i} \tag{3.38}$$

$$\Delta\omega_{x_1-x_2} = \frac{\omega_{b_{x_2}} - \omega_{b_{x_1}}}{\ell n \dfrac{\omega_w - \omega_{b_{x_1}}}{\omega_w - \omega_{b_{x_2}}}} \tag{3.39}$$

$f_{x_1-x_2}$ in Eq.(3.28) is a friction factor for a developing laminar flow through a circular tube. Pressure loss coefficients are shown in Table 1. $\alpha_{x_1-x_2}$ in Eq.(3.32) is a heat transfer coefficient for a thermally developing laminar flow. $\beta_{x_1-x_2}$ in Eq.(3.36) is obtained from Eq.(3.32) on the assumption of analogy between heat and mass transfer. When we solve the algebraic equation, these factor and coefficients are implicitly dealt as constant values. These factor and coefficients are influenced by chemical reactions and are expressed by using dimensionless parameter in the following(5).

$$f = F1(Re,\ X_1/d,\ X_2/d,\ Da,\ Daw) \tag{3.40}$$

$$\alpha = F2(Re,\ Pr,\ X_1/d,\ X_2/d,\ Da,\ Daw) \tag{3.41}$$

$$\beta_i = F3(Re,\ Sc_i,\ X_1/d,\ X_2/d,\ Da_i,\ Daw_i) \tag{3.42}$$

In the calculation, only the parameters of Re, Pr, Sc_i and $(X_2 - X_1)$ are considered to check the calculation method.

3.5 Rate of Chemical Reaction

In the present numerical analysis, the following chemical reactions are considered:

$$C + O_2 \rightarrow CO_2 + 3.934 \times 10^5 \quad (J/mole) \tag{3.a}$$

$$C + \frac{1}{2}O_2 \rightarrow CO + 1.105 \times 10^5 \quad (J/mole) \tag{3.b}$$

$$C + CO_2 \rightarrow 2CO - 1.725 \times 10^5 \quad (J/mole) \tag{3.c}$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 + 5.660 \times 10^5 (J/mole) \tag{3.d}$$

Here, the positive sign represents an exothermic chemical reaction and the negative one an endothermic chemical reaction. It is said that the total chemical reactions of Eqs.(3.a) and (3.b) are the primary ones. The chemical reaction of Eq.(3.c) is called "Boudouard reaction". These three chemical reactions are solid(graphite)/gas reactions. The gas/gas reaction of Eq.(3.d) is the carbon combustion reaction.

The reaction rates of the solid/gas chemical reactions are expressed as follows(6):

$$m_{O_2} = m_C^{(1)} \frac{M_{O_2}}{M_C} \frac{2 + f}{2 + 2f} \tag{3.43}$$

$$m_{CO} = -m_C^{(1)} \frac{M_{CO}}{M_C} \frac{f}{1 + f} - 2m_C^{(2)} \frac{M_{CO}}{M_C} \tag{3.44}$$

$$m_{CO_2} = -m_C^{(1)} \frac{M_{CO_2}}{M_C} \frac{1}{1 + f} + m_C^{(2)} \frac{M_{CO_2}}{M_C} \tag{3.45}$$

$$m_C^{(1)} = -2560 \exp(-\frac{142000}{R_g\ T_K})(\frac{p}{1.013 \times 10^5})^{0.5}(\frac{M}{M_{O_2}} \frac{\omega_{wO_2}}{0.2095})^{0.75} \tag{3.46}$$

$$m_C^{(2)} = -44.5 \exp(-\frac{162714}{R_g\ T_K})\omega_{wCO_2} \tag{3.47}$$

$$f = 800 \exp(-\frac{6200}{T_K}) \tag{3.48}$$

$$Da_{w,i} = \frac{4}{\rho_0 \; u_0} \frac{d_0}{d_k} m_i \tag{3.49}$$

$m_C{}^{(1)}$ and $m_C{}^{(2)}$ are the graphite corrosion rates in the in-pore diffusion control regime. In the present numerical analysis, we deal with the mass transfer control regime and the in-pore diffusion control regime. Thus, we did not give the chemical reaction rates because the chemical reaction control regime lies in the temperature region lower than 400 to 500°C. f of Eq.(3.48) is the generation ratio of carbon monoxide mole fraction to carbon dioxide one.

The following reaction rates in the carbon monoxide combustion reaction are used.

$$R_{CO} = -R^+ \tag{3.50}$$

$$R_{O_2} = -0.5 \; R^+ \frac{M_{O_2}}{M_{CO}} \tag{3.51}$$

$$R_{CO_2} = R^+ \frac{M_{CO_2}}{M_{CO}} \tag{3.52}$$

$$R^+ = k^+ \; \rho (\frac{\rho}{M_{O_2}})^{0.5} \; \omega_{CO} \omega_{O_2}{}^{0.5} \tag{3.53}$$

$$k^+ = 7 \times 10^9 \; \exp(-\frac{199720}{R_g \; T_K}) \tag{3.54}$$

The generation heat due to carbon monoxide combustion is considered in the present code by the equation:

$$Q = 5.660 \times 10^5 \frac{R_{CO_2}}{M_{CO_2}} \tag{3.55}$$

The graphite wall temperature is increased by the graphite/oxygen chemical reactions. The graphite wall temperature after this increase can be used as the input data of the code instead of providing the generation heat of the graphite chemical reactions to the code. Thus, the heat is assumed not to be generated by the graphite/oxygen chemical reactions in the code. The absorption heat due to the graphite/carbon-dioxide chemical reaction was ignored because this chemical reaction occurs scarcely under the present temperature conditions less than 1400°C.

Thermal properties of each gas species and gas mixture in Ref.(7) were used in the present calculation.

3.6 Average Value of Branch

The outlet temperature and outlet mass fraction of the branch would be obtained if the one-dimensional transient basic equation is analytically solved. The basic equation, however, can not be solved because of the non-linearity. Accordingly, the average value of the branch was assumed to be expressed by the inlet and the wall values of the branch as follows:

$$\bar{\Theta} = \Theta_W + (\Theta_X - \Theta_W)\{1 - \exp(-C_T)\} \frac{1}{C_T} \qquad (3.56)$$

$$C_T = \frac{4\ Nu}{\varepsilon_k\ Re\ Pr} \qquad (3.57)$$

$$\bar{\omega}_i = \omega_{W_i} + (\omega_{X_i} - \omega_{W_i})\{1 - \exp(-C_\omega)\} \frac{1}{C_\omega} \qquad (3.58)$$

$$C_\omega = \frac{4\ Sh_i}{\varepsilon_k\ Re\ Sc_i} \qquad (3.59)$$

The above inlet and wall values used were obtained at one iterative step before. The inlet value of the branch is equal to the value at the node to which the inlet of the branch connects.

3.7 Initial and Boundary Conditions

When the primary pipe rupture takes place in the HTTR, the helium gas coolant of about 4 MPa spouts out of the RV to the RCV. After the balance of pressure between the RV and the RCV, the gas mixture of air and helium enters the RV from the RCV by molecular diffusion and by a special type of weak natural convection(8). Then, the natural circulation starts suddenly throughout the reactor after the weak air ingress period continuing for a certain time. We deal with this natural circulation here. Therefore, the flow condition just before the natural circulation should be an initial condition for the calculation in the HTTR. On the other hand, when we carry out the experiment, the test is started by opening the slide valves at the inlet and outlet as shown in Fig. 2. Before the opening, the natural circulation is occurring in only the three parallel channels. The condition of this local natural circulation is the initial condition in the calculation for the experimental apparatus. However, since the objective of the present study is to develop the analytical method, we gave a simple initial condition to the calculation as follows:

(1) Nitrogen gas is filled in the all branches.
(2) All flow rates are equal to zero.
(3) Temperatures of only graphite branches are equal to, for example, 1000°C, and other temperatures are room ones.
(4) All pressures are equal to atmospheric ones.

The following conditions are given as boundary conditions;

(1) Two end branches connect separately to two infinite regions of a gas mixture of nitrogen and oxygen with atmospheric pressure and room temperature.
(2) Wall mass fractions of oxygen, carbon monoxide and carbon dioxide in the graphite branch are obtained by solving the following equations.

$$-\frac{Sh_{O_2}\ \rho^*}{Re\ Sc_{O_2}}\ (\bar{\omega}_{O_2} - \omega_{wO_2}) = \frac{m_{O_2}}{\rho_0\ u_0} \tag{3.60}$$

$$-\frac{Sh_{CO}\ \rho^*}{Re\ Sc_{CO}}\ (\omega_{CO} - \omega_{wCO}) = \frac{m_{CO}}{\rho_0 u_0} \tag{3.61}$$

$$-\frac{Sh_{CO_2}\ \rho^*}{Re\ Sc_{CO_2}}\ (\omega_{CO_2} - \omega_{wCO_2}) = \frac{m_{CO_2}}{\rho_0 u_0} \tag{3.62}$$

It should be noted that the right hand sides of Eqs.(3.60) to (3.62) include wall mass fractions as expressed in Eqs.(3.43) to (3.47). Therefore, first, Eq.(3.60) of the wall mass fraction of oxygen is solved by Newton-Rapson method, then Eq.(6.62) is solved, and last the mass fraction of carbon monoxide can be obtained.

4. Result and Discussion

A steady state calculation was performed under the following conditions;

Graphite wall temperature	: 1000°C
Branch wall temperature	: 20°C
Gas temperature at inlet	: 20°C
Pressure at inlet and outlet	: 1.013×10^5 Pa
Oxygen mass fraction at inlet	: 0.233
Nitrogen mass fraction at inlet	: 0.767

The calculation results of Reynolds numbers in branches, temperatures at nodes, and mass fractions of oxygen, carbon monoxide and carbon dioxide at nodes are shown in Figs. 6-1 to 6-5. The Reynolds numbers in the branches with the same diameter and length differ from one another because of the difference of the bulk gas temperature. The flow rate at the outlet increased a little in comparison with the one at the inlet as shown in Fig. 6-1. This increase of the flow rate results from the gasification of the graphite due to the graphite/gas chemical reactions. The mass fraction of oxygen at the No.2 node (=0.207) is less than that at the No.1 node of the inlet (=0.233) because the flow goes down in the cold branches of the No.14 to No.19. The mass fractions of carbon monoxide and carbon dioxide at the No.2 node are not equal to zero as well as the mass fraction of oxygen at the No.2 node as shown in Figs. 6-4 and 6-5.

A transient calculation was carried out under the same conditions as the above ones. Figures 7 to 10 show the calculation results of the flow rates at the No.5, No.17 and No.27 branches, the gas temperatures at the No.6 and No.18 nodes and the mass fractions of oxygen, carbon monoxide and carbon dioxide at the No.6 and the No.26 nodes, respectively. The abscissa of Figs. 7 to 10 is elapsed time. The time increment was 0.2 seconds in the calculation. It is found that the values calculated reach steady state after about 5 seconds. The results in the steady state calculation agreed with those of steady state in the transient calculation. In these figures the overshooting is observed at the initial stage shorter than few seconds of the elapsed time.

The calculation results will be compared with the corresponding experimental results to verify the method of the numerical analysis.

5. Concluding Remarks

The flow network computer code was developed to calculate heat, mass and momentum transfer in a natural circulation of a multicomponent gas mixture with graphite chemical reaction due to air ingress. The entering flow rate, flow rates distributed to the parallel channels, generation volume of carbon monoxide and corrosion volume of the graphite were predicted by the present code. It was found that the numerical calculation method used in the code was basically effective for the analysis of heat, mass and momentum transfer in the gas mixture flow with solid(graphite)/gas(oxygen or carbon dioxide) and gas/gas(carbon monoxide/oxygen) chemical reactions.

We have already carried out the experiments on the graphite corrosion at high temperature in the experimental apparatus as shown in Fig. 2. The results calculated by the code will be compared with those obtained in the experiment.

References

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(8) M. Hishida and T. Takeda, Study on Air Ingress during An Early Stage of A Primary-pipe Rupture Accident of A High-temperature Gas-cooled Reactor, Nucl. Eng. Des., 126 (1991), 175.

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We have already carried out the experiments on the graphite corrosion at high temperature in the experimental apparatus as shown in Fig. 2. The results calculated by the code will be compared with those obtained in the experiment.

References

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(6) M. Ogawa, Mass Transfer with Graphite Oxidation in A Gas Mixture Laminar Flow through A Circular Tube, J. Atomic Energy Soc. Japan, to be published.

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Table 1 Dimensions of branches and Pressure loss coefficients

Branch number	Length (m)	Diameter (m)	Θ (deg)	Pressure coefficient
1	0.691	0.0549	0	1.5
2	0.7	0.0492	90	1.5
3	0.7025	0.0549	0	0
4	0.7025	0.0549	0	0
5	0.7	0.0549	0	0
6	1.085	0.0549	0	0
7	0.7	0.0492	90	1.5
8	0.7	0.0492	90	1.5
9	0.7025	0.0549	0	0
10	0.7025	0.0549	0	0
11	0.7	0.0549	0	0
12	1.085	0.0549	0	0
13	0.7	0.0492	90	1.5
14	0.7	0.0492	90	1.5
15	0.7975	0.0549	0	0
16	0.7975	0.0549	0	0
17	0.7975	0.0549	0	0
18	0.7975	0.0549	0	0
19	0.7	0.0492	90	1.5
20	0.246	0.0549	0	1.0
21	0.35	0.0549	90	1.0
22	0.688	0.0549	180	0
23	0.688	0.0549	180	0
24	0.688	0.0549	180	0
25	0.688	0.0549	180	0
26	0.688	0.0549	180	0
27	0.688	0.0549	180	0

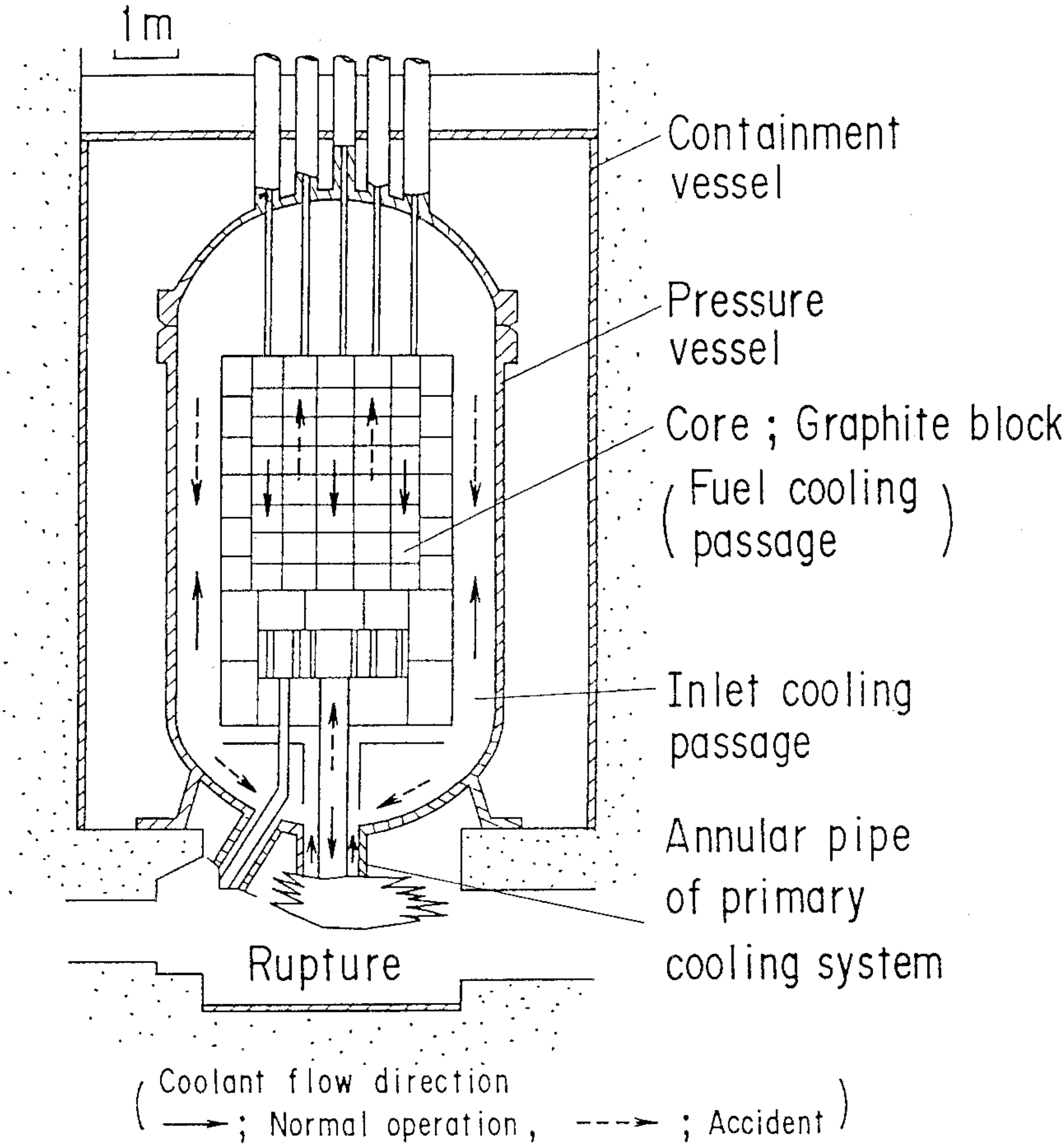

Fig. 1 Cross-sectional view of HTTR.

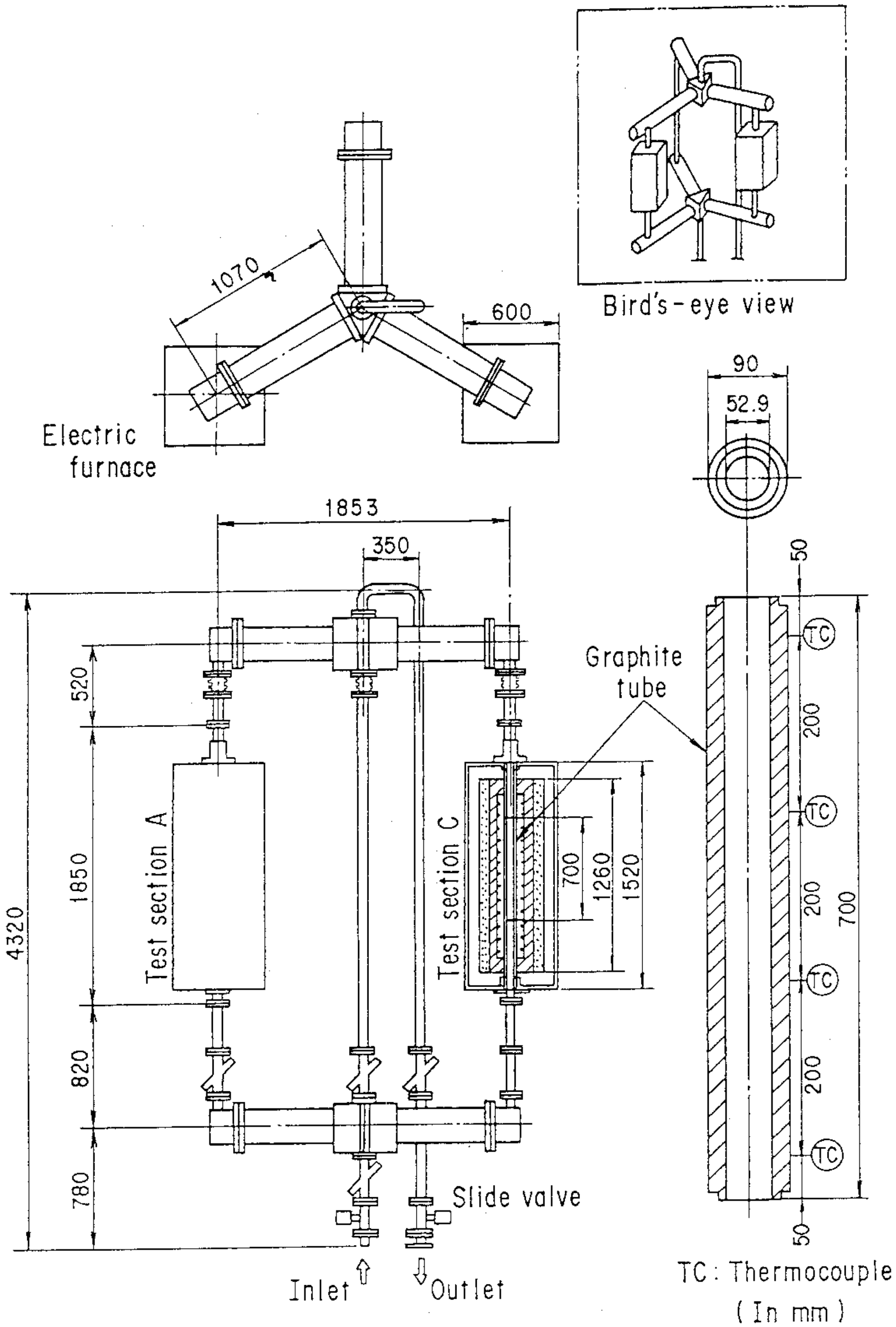

Fig. 2 Experimental apparatus for heat, mass and momentum transfer in a natural convection with graphite chemical reactions.

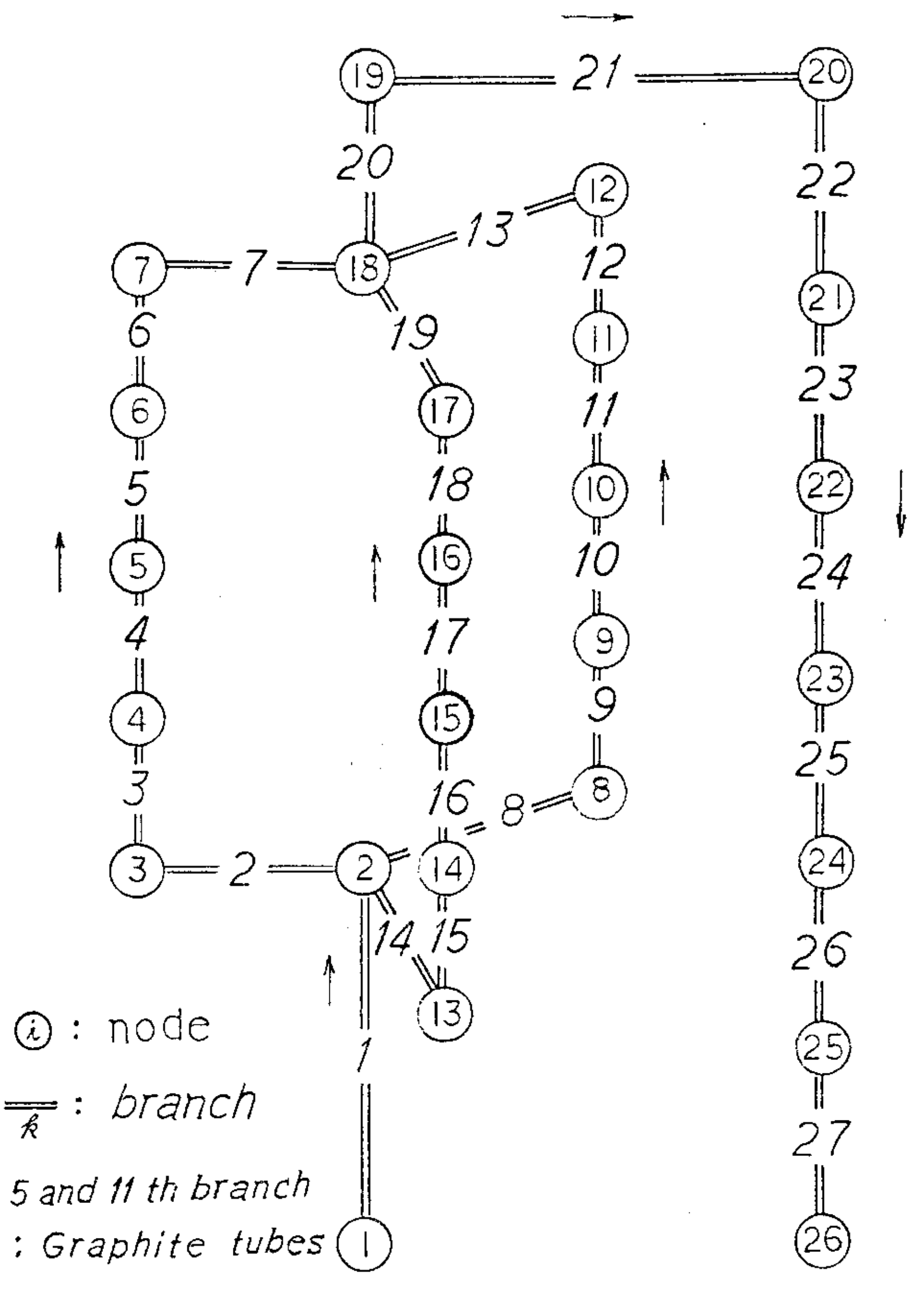

Fig. 3 Correction of branches and nodes in flow network corresponding to flow channels of experimental apparatus

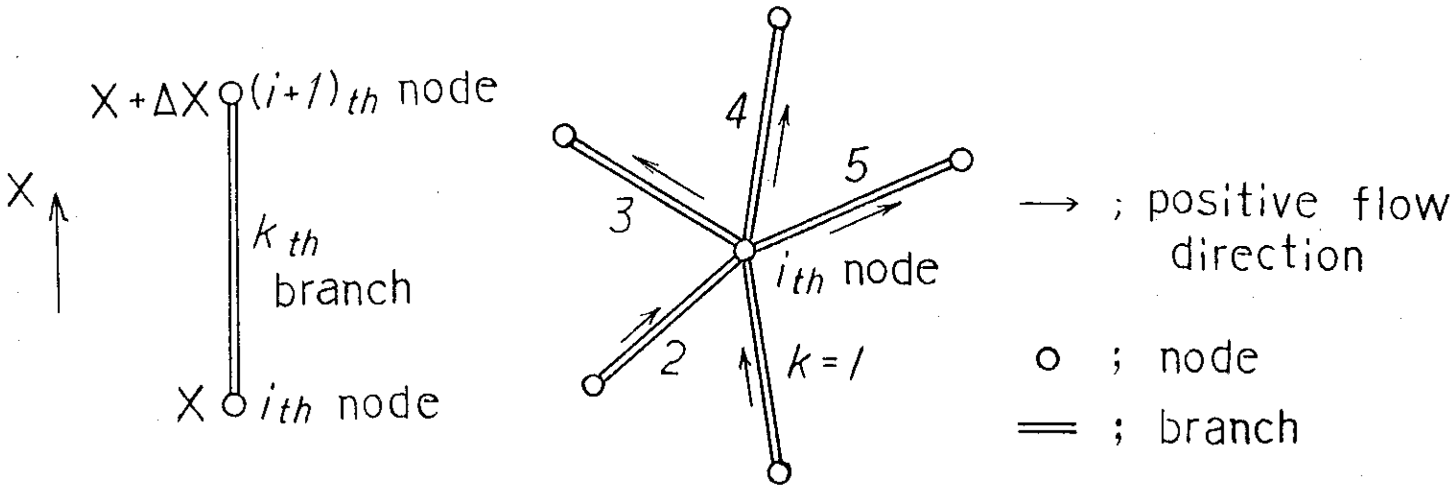

Fig. 4 An example of branch-node connection.

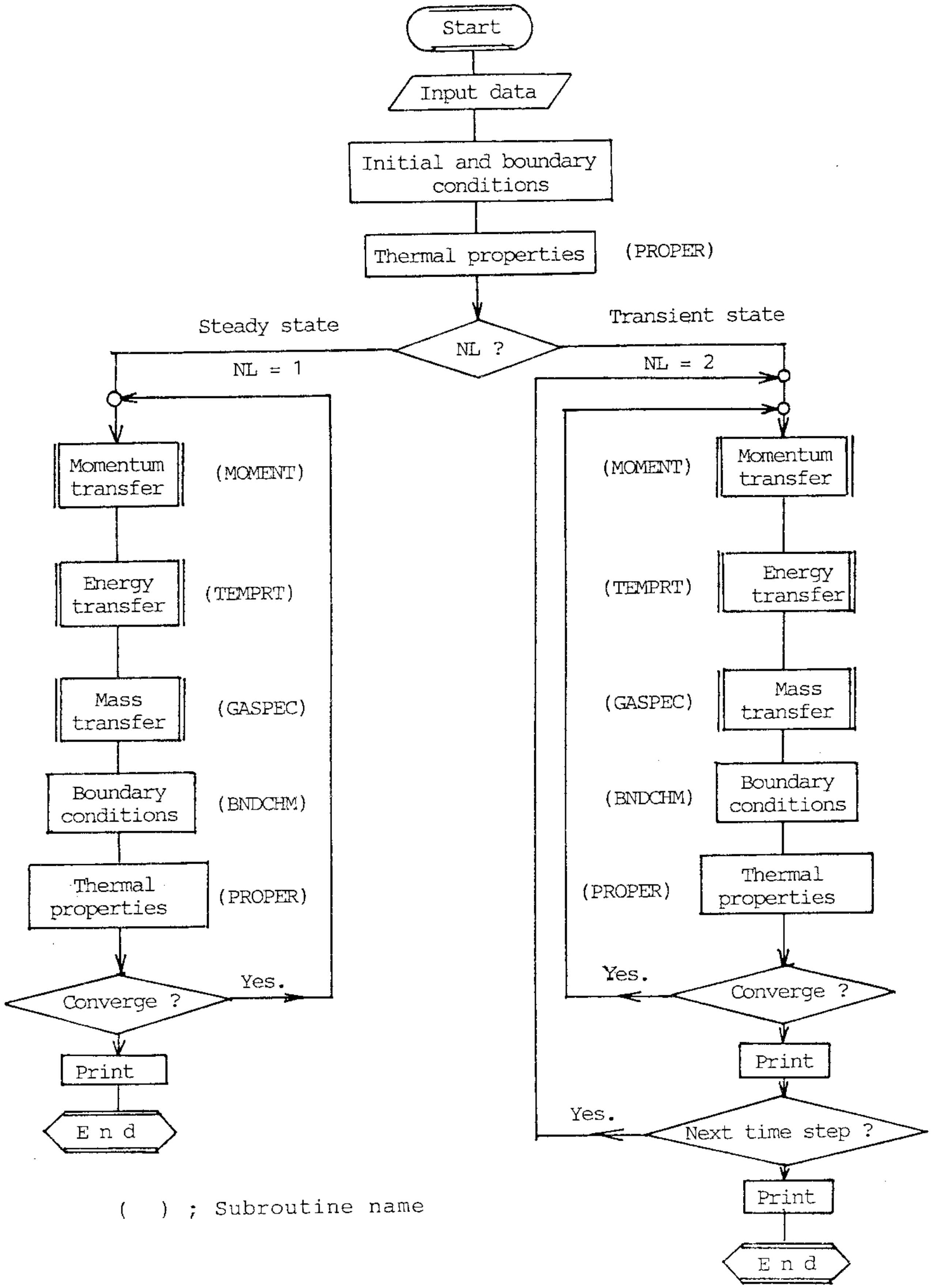

Fig. 5 Flow diagram of computer program.

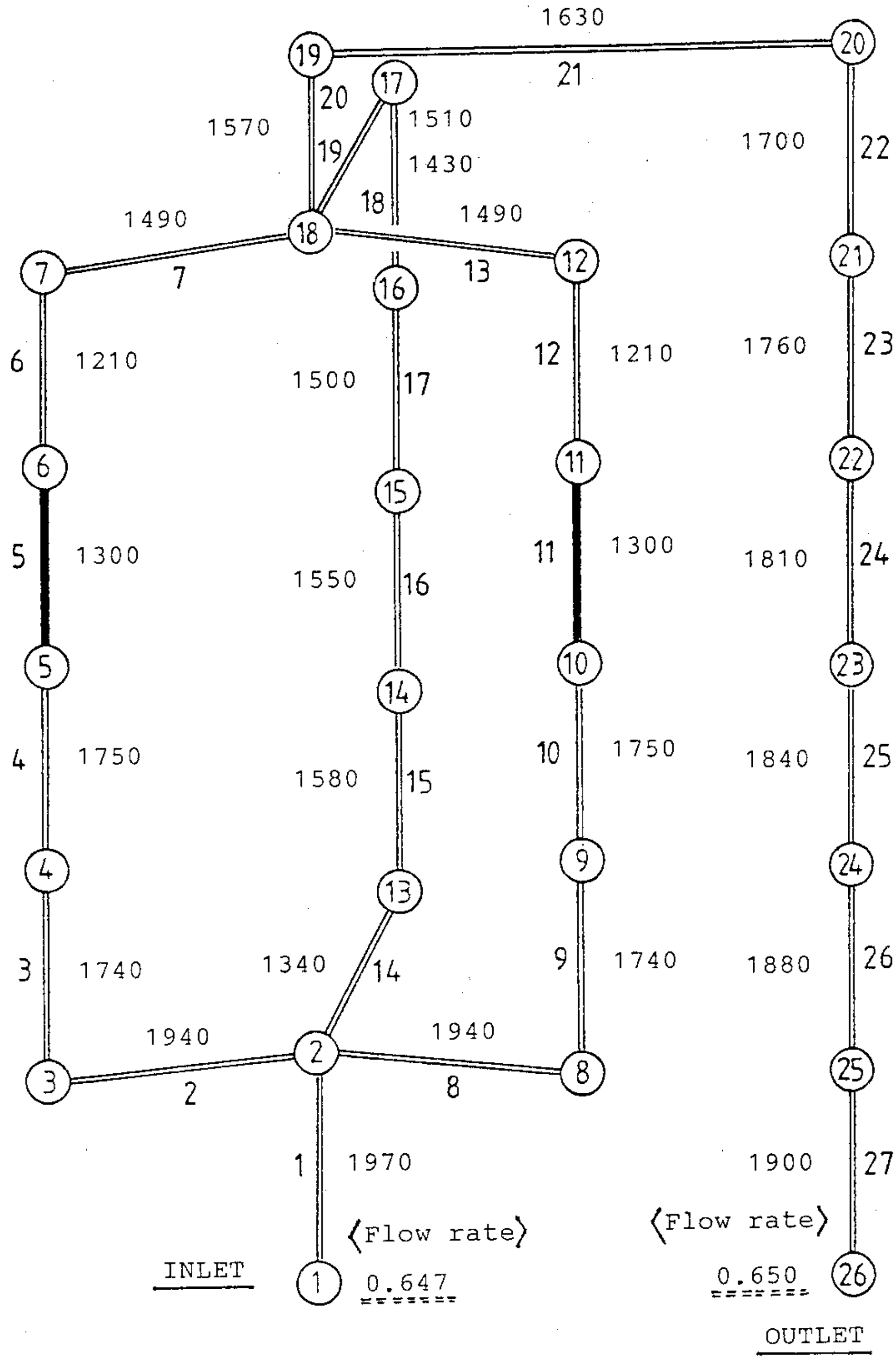

Fig. 6-1 Reynolds numbers of branches in steady state.

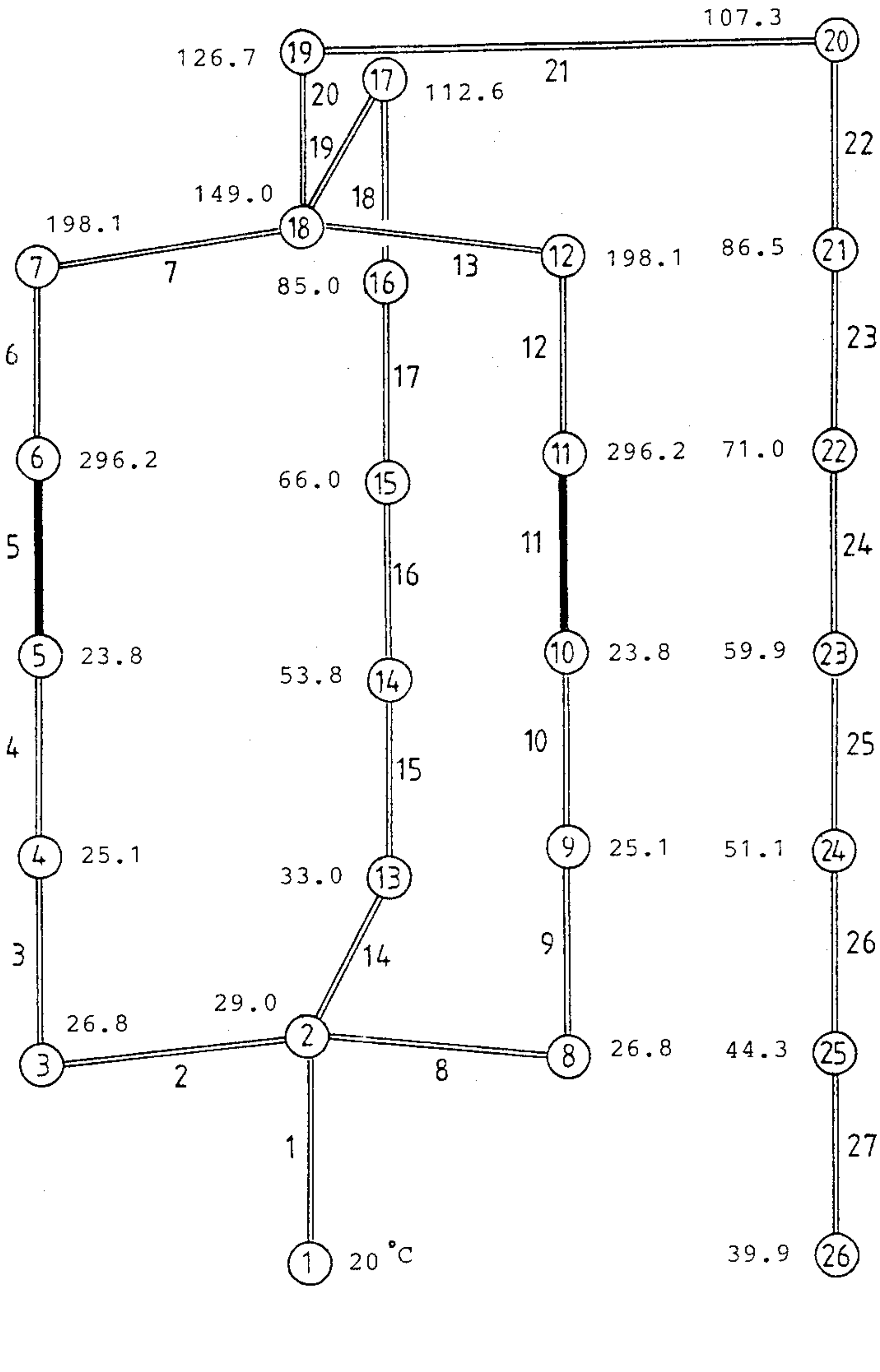

Fig. 6-2 Temperatures at nodes in steady state.

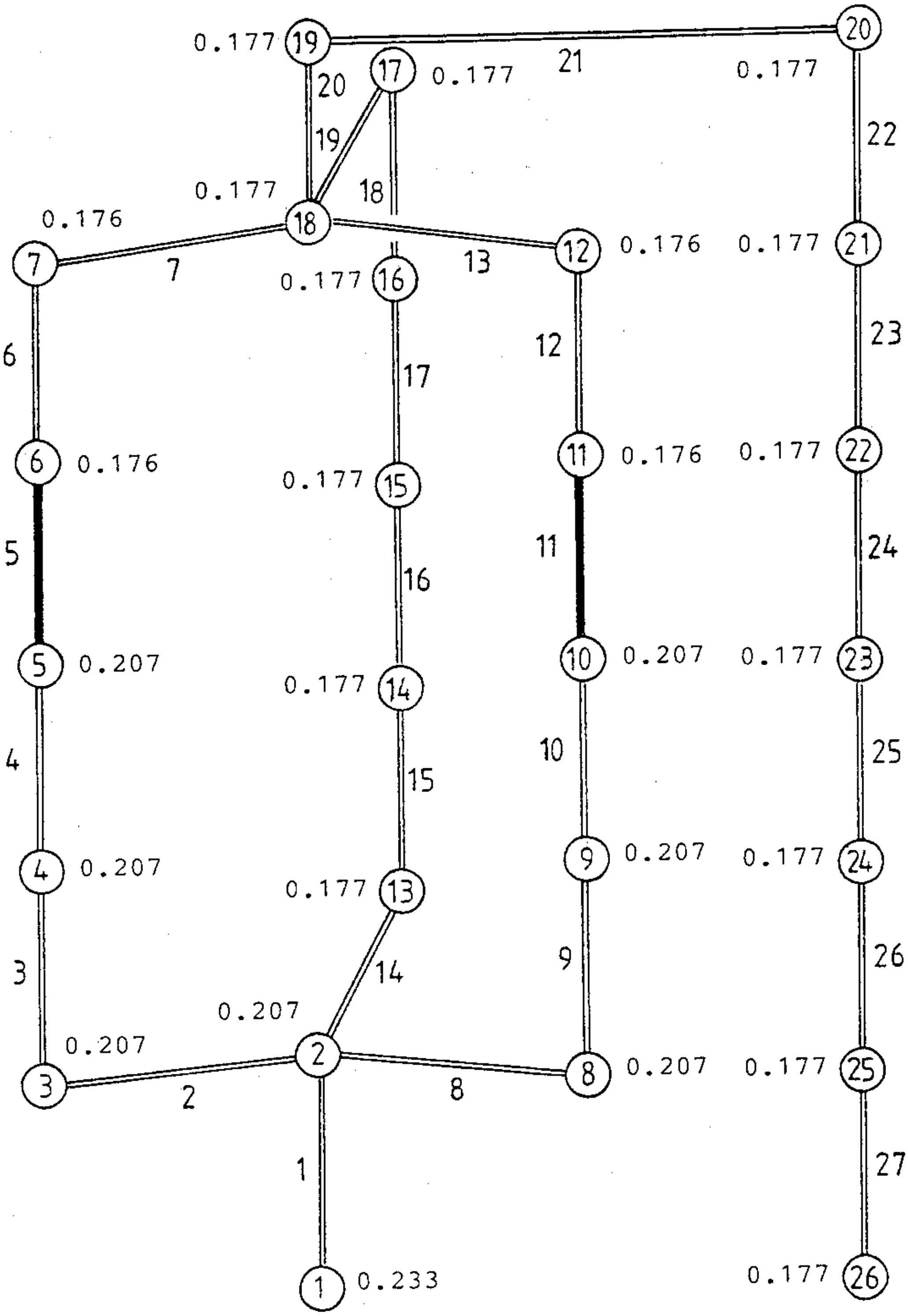

Fig. 6-3 Mass fractions of oxygen at nodes in steady state.

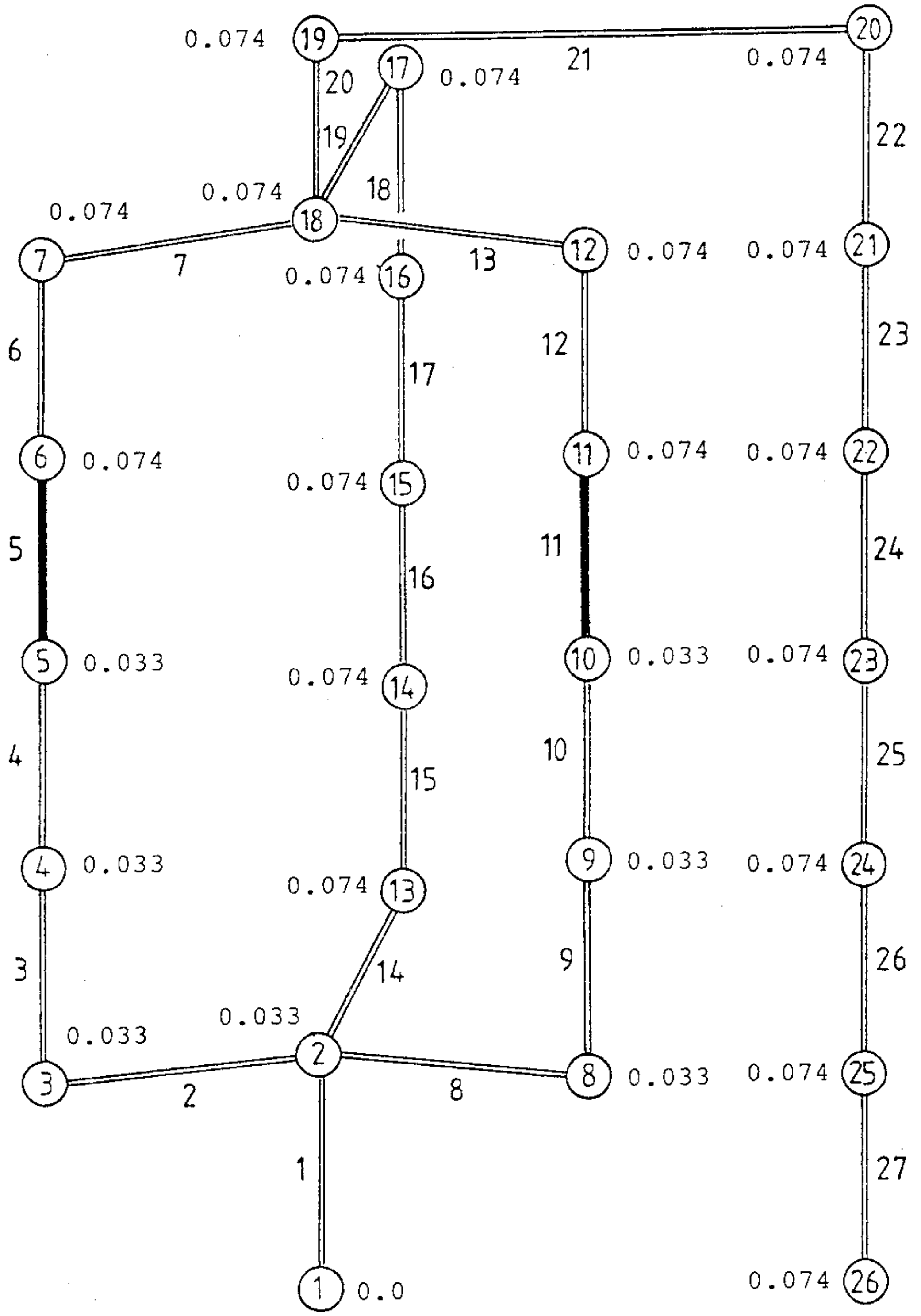

Fig. 6-4 Mass fractions of carbon monoxide at nodes in steady state.

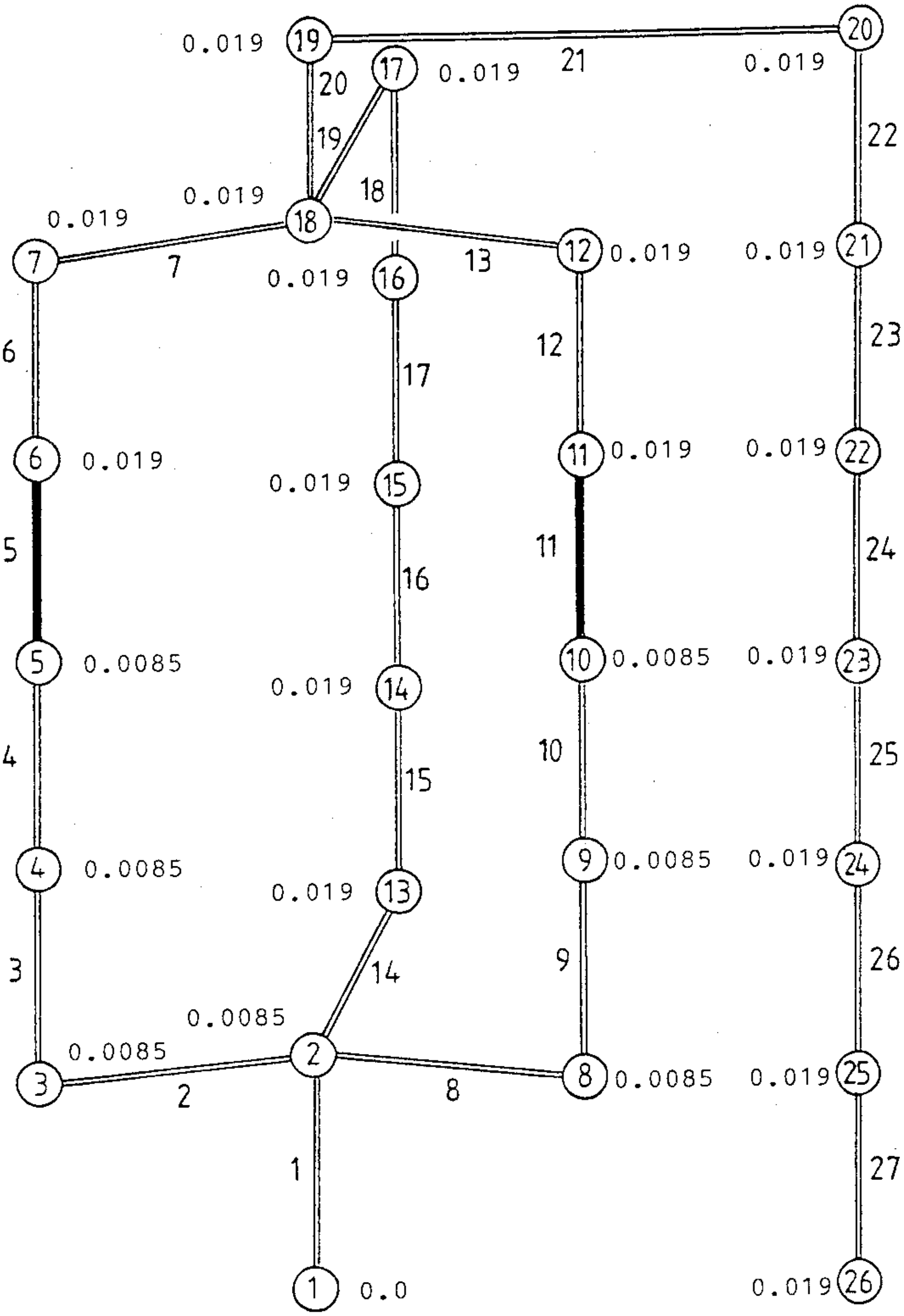

Fig. 6-5 Mass fractions of carbon dioxide at nodes in steady state.

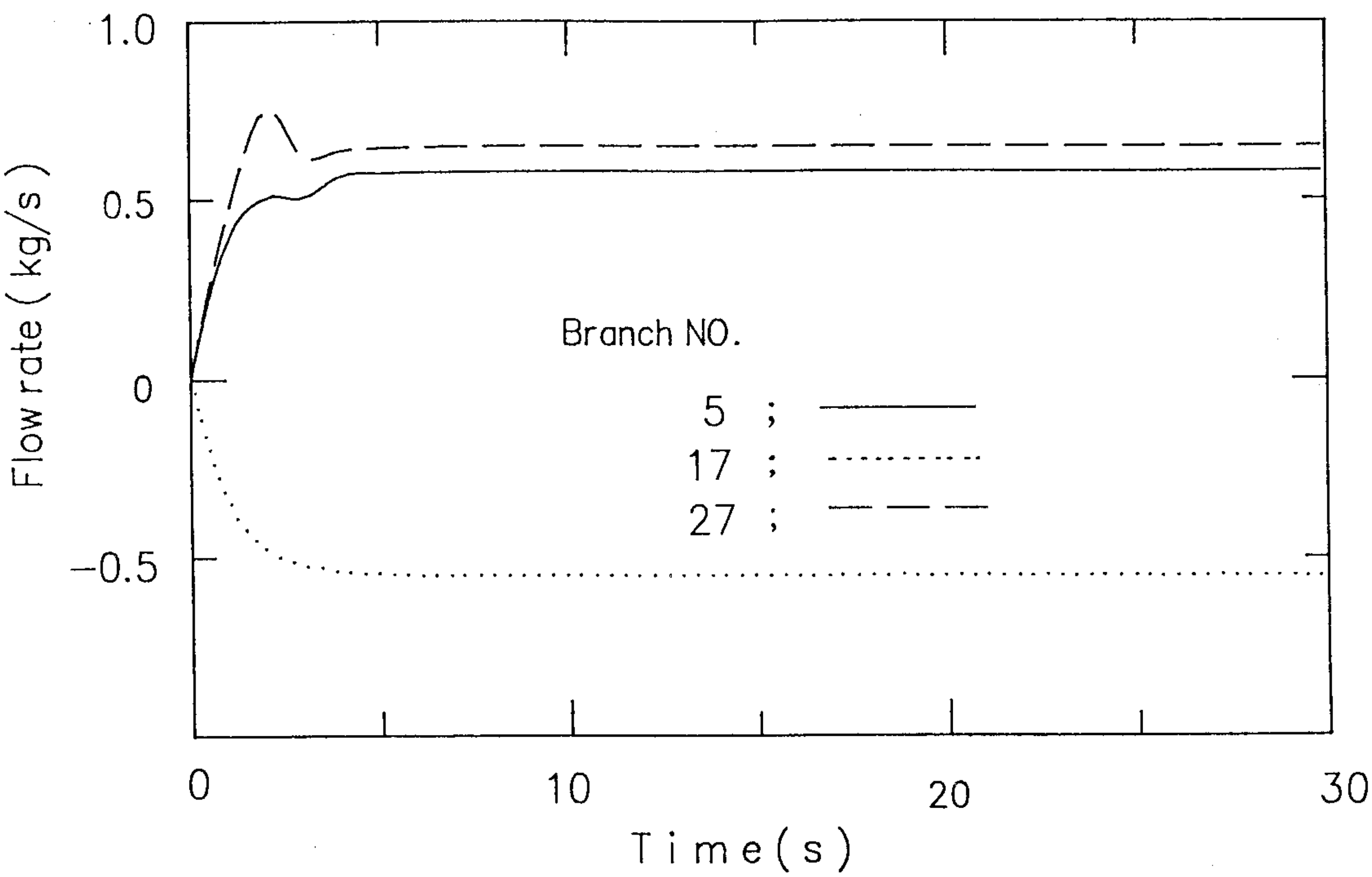

Fig. 7 Flow rates at the No.5, No.17 and No.27 branches in the transient calculation.

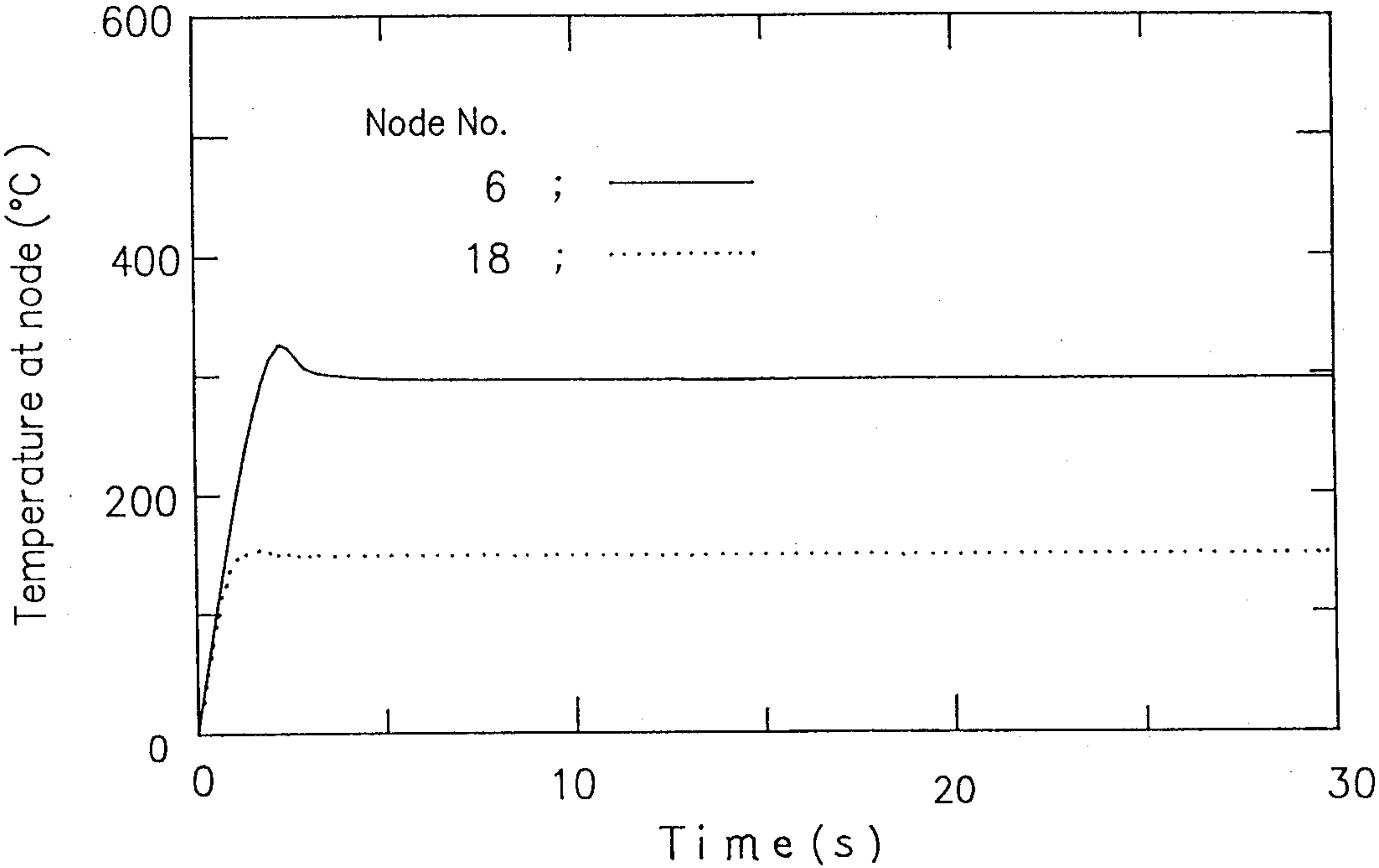

Fig. 8 Gas temperatures at the No.6 and No.18 nodes in the transient calculation.

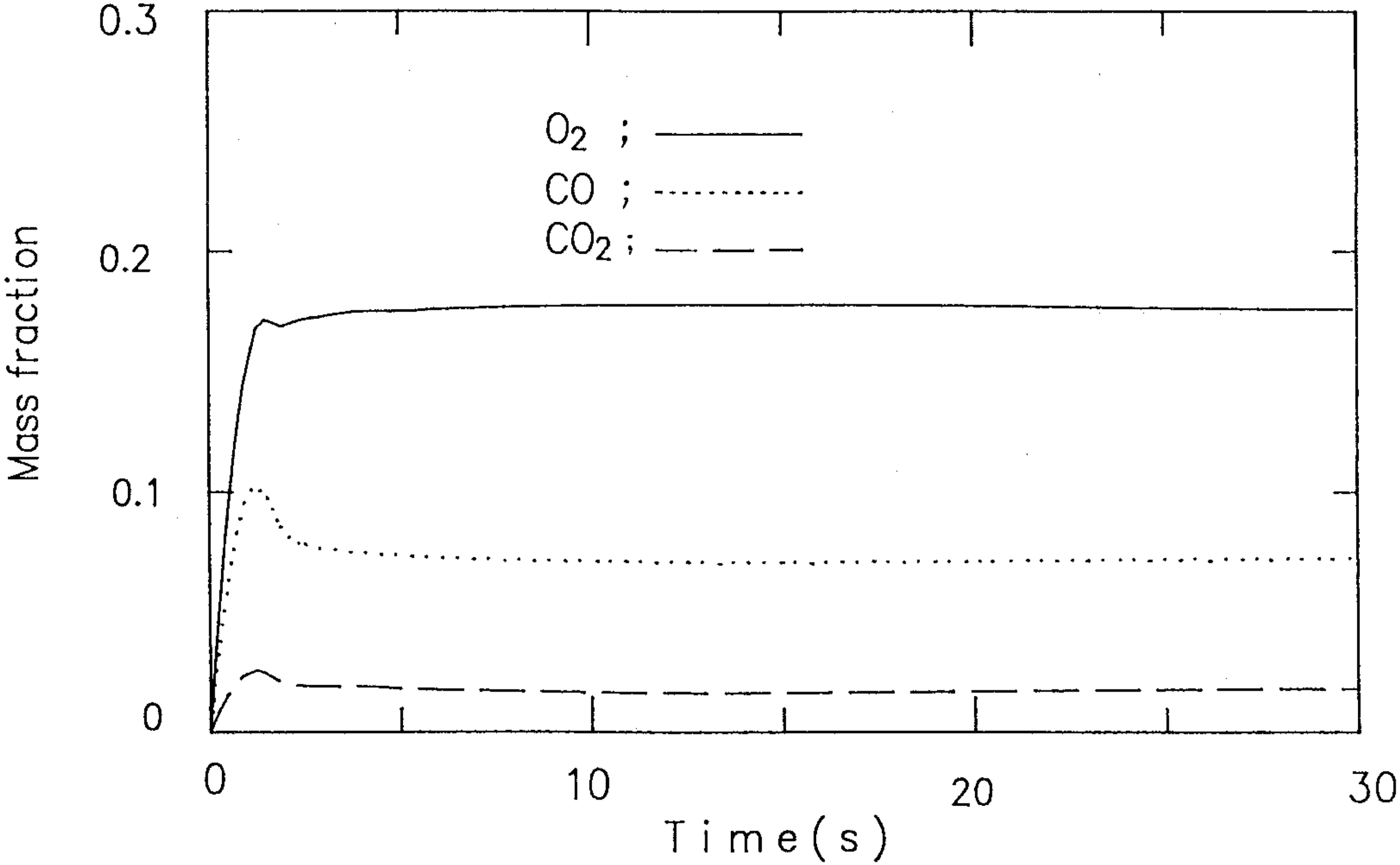

Fig. 9 Mass fractions at the No.6 node in the transient calculation.

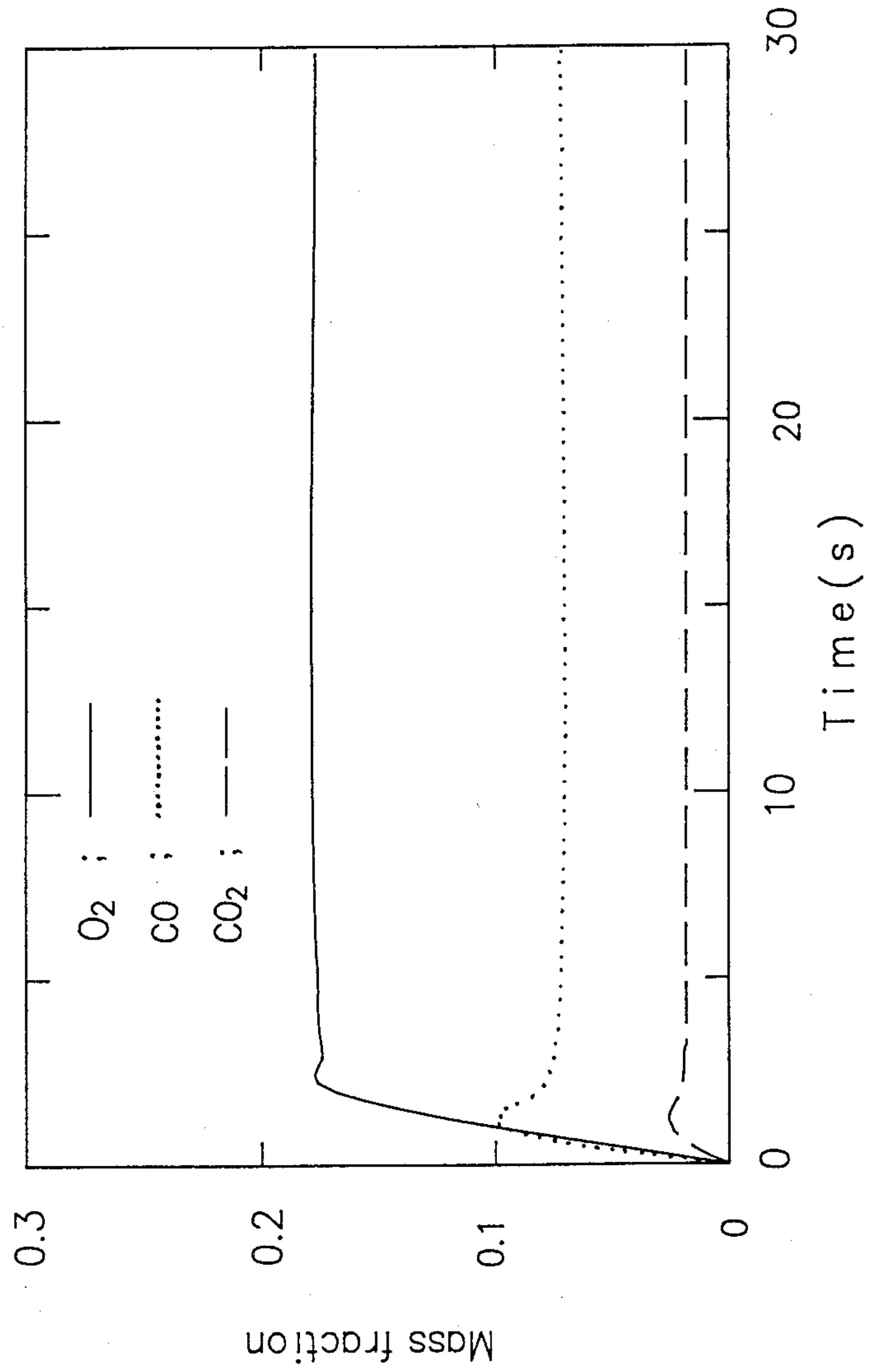

Fig. 10 Mass fraction at the No.26 node in the transient calculation.

APPENDIX Computer Program

```
      FORTRAN77 EX    V12L10                DATE 92-09-21  TIME 20:42:03

C
C***********************************************************************
C***********************************************************************
C******                                                           *****
C******      COMPUTER CODE FOR NUMERICAL ANALYSIS ON HEAT, MASS    *****
C******        AND MOMENTUM TRANSFER IN A MULTI-COMPONENT GAS      *****
C******           MIXTURE WITH GRAPHITE CHEMICAL REACTIONS         *****
C******                                                           *****
C******                                         MARCH 27, 1992    *****
C******                                                           *****
C***********************************************************************
C***********************************************************************
C
C   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C   +               ----------------------------------                +
C   +               ---   DEFINITION OF VARIABLES   ---               +
C   +               ----------------------------------                +
C   +                                                                 +
C   +    N     = THE NUMBER OF NODES                                  +
C   +    M     = THE NUMBER OF BRANCHES                               +
C   +    K     = THE NUMBER OF GAS SPECIES ; HE=1,O2=2,CO=3,CO2=4,N2=5 +
C   +    J     = ITERATION TIMES                                      +
C   +    DTI   = INCREMENT OF TIME STEP                               +
C   +    DT    = INCREMENT OF TIME STEP                               +
C   +    TIME  = ELAPSED TIME OF CALCULATION                          +
C   +    NL    = CONTROL CONSTANT FOR CALCULATIONS                    +
C   +                                                                 +
C   +    H      = LENGTH OF BRANCH                                    +
C   +    D      = HYDRAULIC DIAMETER                                  +
C   +    Y      = PRESSURE LOSS FACTOR                                +
C   +    F      = FRICTION FACTOR                                     +
C   +    NNI(K)= THE NUMBER OF THE NODE CONNECTING TO KTH BRANCH INLET +
C   +    NNO(K)= THE NUMBER OF THE NODE CONNECTING TO KTH BRANCH OUTLET +
C   +    CAT    = VERTICALITY OF BRANCH                               +
C   +                                                                 +
C   +    TN1  = TEMPERATURE OF GAS AT NODE (OLD)                      +
C   +    TN2  = TEMPERATURE OF GAS AT NODE (NEW)                      +
C   +    TTN  = TEMPERATURE OF GAS AT NODE                            +
C   +    TTNT = TEMPERATURE OF GAS AT NODE IN TIME ITERATION          +
C   +    TO1  = TEMPERATURE OF GAS AT BRANCH OUTLET (OLD)             +
C   +    TO2  = TEMPERATURE OF GAS AT BRANCH OUTLET (NEW)             +
C   +    TTO  = TEMPERATURE OF GAS AT BRANCH OUTLET                   +
C   +    TTOT = TEMPERATURE OF GAS AT BRANCH OUTLET IN TIME ITERATION +
C   +    TA1  = AVERAGE TEMPERATURE OF GAS IN BRANCH (OLD)            +
C   +    TA2  = AVERAGE TEMPERATURE OF GAS IN BRANCH (NEW)            +
C   +    TWA  = AVERAGE TEMPERATURE OF WALL                           +
C   +    TTA  = AVERAGE TEMPERATURE OF GAS IN BRANCH                  +
C   +    TTAT = AVERAGE TEMPERATURE OF GAS IN BRANCH IN TIME ITERATION +
C   +                                                                 +
C   +    P1   = PRESSURE OF NODE (OLD)                                +
C   +    P2   = PRESSURE OF NODE (NEW)                                +
C   +    PP   = PRESSURE OF NODE                                      +
C   +    PPT  = PRESSURE OF NODE IN TIME ITERATION                    +
C   +    PX1  = DIMENTIONLESS PRESSURE OF NODE (OLD)                  +
C   +    PX2  = DIMENTIONLESS PRESSURE OF NODE (NEW)                  +
C   +    PA1  = AVERAGE PRESSURE OF BRANCH (OLD)                      +
C   +    PA2  = AVERAGE PRESSURE OF BRANCH (NEW)                      +
C   +                                                                 +
C   +    WN1  = CONCENTRATION OF GAS AT NODE (OLD)                    +
C   +    WN2  = CONCENTRATION OF GAS AT NODE (NEW)                    +
```

```
      FORTRAN77 EX    V12L10                    DATE 92-09-21   TIME 20:42:03
C  +     WWN  = CONCENTRATION OF GAS AT NODE                                  +
C  +     WWNT = CONCENTRATION OF GAS AT NODE IN TIME ITERATION                +
C  +     WO1  = CONCENTRATION OF GAS AT BRANCH OUTLET (OLD)                   +
C  +     WO2  = CONCENTRATION OF GAS AT BRANCH OUTLET (NEW)                   +
C  +     WWO  = CONCENTRATION OF GAS AT BRANCH OUTLET                         +
C  +     WWOT = CONCENTRATION OF GAS AT BRANCH OUTLET IN TIME ITERATION       +
C  +     WA1  = AVERAGE CONCENTRATION OF GAS IN BRANCH (OLD)                  +
C  +     WA2  = AVERAGE CONCENTRATION OF GAS IN BRANCH (NEW)                  +
C  +     WAA  = AVERAGE CONCENTRATION OF GAS IN BRANCH                        +
C  +     WAAT = AVERAGE CONCENTRATION OF GAS IN BRANCH IN TIME ITERATION+
C  +     WWA  = AVERAGE CONCENTRATION OF GAS AT WALL                          +
C  +                                                                          +
C  +     GA1  = AVERAGE MASS FLOW RATE IN BRANCH (OLD)                        +
C  +     GA2  = AVERAGE MASS FLOW RATE IN BRANCH (NEW)                        +
C  +     GX1  = DIMENTIONLESS AVERAGE MASS FLOW RATE IN BRANCH (OLD)          +
C  +     GX2  = DIMENTIONLESS AVERAGE MASS FLOW RATE IN BRANCH (NEW)          +
C  +     GG   = AVERAGE MASS FLOW RATE IN BRANCH                              +
C  +     GGT  = AVERAGE MASS FLOW RATE IN BRANCH IN TIME ITERATION            +
C  +     GM   = MASS FLUX OF EACH GAS BY GRAPHITE CHEMICAL REACTIONS          +
C  +     GM1  = MASS FLUX OF CARBON BY GRAPHITE CHEMICAL REACTIONS            +
C  +                                                                          +
C  +     DI   = DIFFUSION COEFFICIENT                                         +
C  +     CP   = SPECIFIC HEAT OF GAS MIXTURE                                  +
C  +     CPN  = SPECIFIC HEAT OF GAS MIXTURE AT NODE                          +
C  +     CPO  = SPECIFIC HEAT OF GAS MIXTURE AT BRANCH OUTLET                 +
C  +     MU   = VISCOSITY OF GAS MIXTURE                                      +
C  +     LAM  = THERMAL CONDUCTIVITY OF GAS MIXTURE                           +
C  +     DEI  = DENSITY OF GAS MIXTURE AT NODE                                +
C  +     DEO  = DENSITY OF GAS MIXTURE AT BRANCH OUTLET                       +
C  +     DEA1 = AVERAGE DENSITY OF GAS MIXTURE IN BRANCH                      +
C  +     DEAT = AVERAGE DENSITY OF GAS MIXTURE IN BRANCH IN TIME              +
C  +            ITERATION                                                     +
C  +                                                                          +
C  +     RE   = REYNOLDS NUMBER                                               +
C  +     GR   = GRASHOF NUMBER                                                +
C  +     NU   = NUSSELT NUMBER                                                +
C  +     SC   = SCHMIDT NUMBER                                                +
C  +     SH   = SHERWOOD NUMBER                                               +
C  +                                                                          +
C  +     BAT  = MASS TRANSFER COEFFICIENT                                     +
C  +     SI   = PRODUCT MASS BY CHEMICAL REACTIONS                            +
C  +     Q    = REACTION HEAT                                                 +
C  +                                                                          +
C  +     C(1) = PRESSURE (=1.0E5 PA)                                          +
C  +     C(2) = TEMPRERATURE (=20 C)                                          +
C  +     C(3) = DENSITY                (N2,    20 C,   0.1 MPA)               +
C  +     C(4) = DENSITY                (N2,  1000 C,   0.1 MPA)               +
C  +     C(5) = VISCOSITY              (N2,    20 C,   0.1 MPA)               +
C  +     C(6) = THERMAL CONDUCTIVITY   (N2,    20 C,   0.1 MPA)               +
C  +     C(7) = SPECIFIC HEAT          (N2,    20 C,   0.1 MPA)               +
C  +     C(8) = DIFFUSION FACTOR       (N2,    20 C,   0.1 MPA)               +
C  +     C(9) = DIFFUSION FACTOR       (O2,    20 C,   0.1 MPA)               +
C  +     C(10)= DIFFUSION FACTOR       (CO,    20 C,   0.1 MPA)               +
C  +     C(11)= DIFFUSION FACTOR       (CO2,   20 C,   0.1 MPA)               +
C  +     C(12)= DIFFUSION FACTOR       (N2,    20 C,   0.1 MPA)               +
C  +     C(13)= KINEMATIC VISCOSITYL   (N2,    20 C,   0.1 MPA)               +
C  +     MOLW = MOLAR MASS OF GAS                                             +
C  +                                                                          +
C  ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
```

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            C
00000001          IMPLICIT REAL*8 (A-H,O-Z)
00000002          PARAMETER ( N=26, M=27, K=5, J=200 )
            C
00000003          DIMENSION H(M), D(M), Y(M), F(M), CAT(M),
                 *           TI1(M), TI2(M), TO1(M), TO2(M), TA1(M), TA2(M),
                 *           TN1(N), TN2(N), TWA(M), TTAT(M),
                 *           GA1(M), GA2(M), GA(M), GGT(M), GM1(M),
                 *           RE(M), GR(M), PR(M), SC(M,K), SH(M,K), Q(M),
                 *           DI(M,K), CP(M), CPT(M), CPO(M), CPN(M), DEI(M), DEO(M),
                 *           DEA1(M), DEAT(M),
                 *           AVEMOL(M), C(13),
                 *           P1(N), P2(N), PN1(N), PN2(N), PA1(M), PA2(M),
                 *           PP(N), PPT(N), PAT(M),
                 *           WI1(M,K), WI2(M,K), WO1(M,K), WO2(M,K), WA1(M,K),
                 *           WA2(M,K), WN1(N,K), WN2(N,K), WAAT(M,K), WWA(M,K),
                 *SCH(K), OMGB(K), OMGW(K), AMOL(K+1), CC(13),
                 *TTN(N), TTO(M), TTA(M), TTOT(M), TTNT(N),
                 *WAA(M,K),WWN(N,K),WWO(M,K),WWOT(M,K),WWNT(N,K),GG(M)
00000004          REAL*8 NNI(M),NNO(M),MU(M),LAM(M),NU(M),MOLW(K+1)
            C
00000005          COMMON/SIZE/H,D,Y,F,NNI,NNO,CAT,DT
                 *      /TEMP/TI1,TI2,TO1,TO2,TA1,TA2,TN1,TN2,TWA,TTAT
                 *      /PRES/P1,P2,PN1,PN2,PA1,PA2,PP,PPT,PAT
                 *      /COMP/WI1,WI2,WO1,WO2,WA1,WA2,WN1,WN2,WAAT,WWA
                 *      /FLOW/GA1,GA2,GA,GGT,GM1
                 *      /QUAL/DI,CP,CPT,CPO,CPN,MU,LAM,DEI,DEO,DEA1,DEAT
                 *      /MLWG/MOLW,AVEMOL,C
                 *      /REFE/RE,GR,PR,NU,SC,SH,Q
            C
00000006          DATA AMOL/4.003E-3, 32.000E-3, 28.010E-3, 44.010E-3, 28.016E-3,
                 *           12.010E-3/
                 *    CC/1.013E+5, 293.15, 1.1960, 3.8320E-2, 1.8497E-5, 25.7E-3,
                 *      1.006E3, 6.879E-5, 1.992E-5, 1.973E-5, 1.501E-5,
                 *      1.974E-5, 1.546572E-5/
00000007          DO 20 I=1,K+1
00000008 20       MOLW(I) = AMOL(I)
00000009          DO 30 I=1,13
00000010 30       C(I)    = CC(I)
            C
            C****************** INPUT DATA ****************************************
            C
00000011          READ(5,*) TIME, DTI, NL
00000012          READ(5,*) (NNI(I),I=1,M-3)
00000013          READ(5,*) (NNI(I),I=M-2,M)
00000014          READ(5,*) (NNO(I),I=1,M-7)
00000015          READ(5,*) (NNO(I),I=M-6,M)
00000016          READ(5,*) (P1(I),I=1,N)
00000017          READ(5,*) (H(I),I=1,M-9)
00000018          READ(5,*) (H(I),I=M-8,M)
00000019          READ(5,*) (D(I),I=1,M)
00000020          READ(5,*) (CAT(I),I=1,M)
00000021          READ(5,*) (Y(I),I=1,M)
00000022          READ(5,*) (TN1(I),I=1,N)
00000023          READ(5,*) (TWA(I),I=1,M)
00000024          DO 10 JJ=1,K
00000025          READ(5,*) (WA1(I,JJ),I=1,M)
00000026 10       CONTINUE
00000027          DO 11 JJ=1,K
00000028          READ(5,*) (WN1(I,JJ),I=1,N)
```

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00000029 11     CONTINUE
         C
00000030        WRITE(6,6100) TIME, DTI, NL
00000031        WRITE(6,6000) (NNI(I),I=1,M)
00000032        WRITE(6,6000) (NNO(I),I=1,M)
00000033        WRITE(6,6000) (P1(I),I=1,N)
00000034        WRITE(6,6000) (H(I),I=1,M)
00000035        WRITE(6,6000) (D(I),I=1,M)
00000036        WRITE(6,6000) (CAT(I),I=1,M)
00000037        WRITE(6,6000) (Y(I),I=1,M)
00000038        WRITE(6,3130) (I,TN1(I),I=1,N)
00000039        WRITE(6,3135) (I,TWA(I),I=1,M)
00000040        DO 12 JJ=1,K
00000041        WRITE(6,3150) JJ, (I,WN1(I,JJ),I=1,N)
00000042 12     WRITE(6,3180)      (I,WA1(I,JJ),I=1,M)
         C
00000043  6000 FORMAT(1H0,10(1PE12.5,1X),/,1X,10(E12.5,1X),/,1X,10(E12.5,1X))
00000044  6100 FORMAT(1H0,30('='),'    INPUT DATA    ',75('='),/,
              *  '        TIME = ',F8.3,' (SEC),    DT = ',F7.3,' (SEC)',
              *  '    NL = ',I1,'    ( NL=1 ; STEADY STATE,      NL=2 ; ',
              *  'TRANSIENT STATE. )' )
         C
         C*************** INITIAL VALUES ***************************************
         C
00000045        DO 100   I=1,M
00000046        P2(NNI(I))=0.0
00000047        P2(NNO(I))=0.0
00000048        GA2(I)=0.0
00000049        TA2(I)=0.0
00000050        TO2(I)=0.0
00000051        TO1(I)=TWA(I)
00000052        TA1(I)=0.5*(TN1(NNI(I))+TO1(I))
00000053        PA1(I)=0.5*(P1(NNI(I))+P1(NNO(I)))
00000054        PAT(I)=PA1(I)
00000055        GA1(I)=0.100
00000056        GG(I)=GA1(I)
00000057        GGT(I)=GA1(I)
00000058        TTO(I)=TO1(I)
00000059        TTOT(I)=TTO(I)
00000060        TTA(I)=TA1(I)
00000061        TTAT(I)=TA1(I)
00000062 100    CONTINUE
00000063        P2(NNI(1))=C(1)
00000064        DO 110 I=1,N
00000065        PP(I)=P1(I)
00000066        PPT(I)=PP(I)
00000067        TN2(I)=0.0
00000068        TTN(I)=TN1(I)
00000069        TTNT(I)=TTN(I)
00000070 110    CONTINUE
00000071        DO 120 I=1,M
00000072        DO 120  JJ=1,K
00000073        WO2(I,JJ)=0.0
00000074        WA2(I,JJ)=0.0
00000075        WWA(I,JJ)=WA1(I,JJ)
00000076        WO1(I,JJ)=WA1(I,JJ)
00000077        WWO(I,JJ)=WA1(I,JJ)
00000078        WAA(I,JJ)=WA1(I,JJ)
00000079        WWOT(I,JJ)=WWO(I,JJ)
00000080        WAAT(I,JJ)=WAA(I,JJ)
```

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```
 120  CONTINUE
      DO 130 I=1,N
      DO 130 JJ=1,K
      WN2(I,JJ)=0.0
      WWN(I,JJ)=WN1(I,JJ)
      WWNT(I,JJ)=WN1(I,JJ)
 130  CONTINUE
C
      CALL PROPER
C
      NSORT = 1
      IF ( NL.GE.2 )  NSORT = 2
      IF(NL.EQ.1) GO TO 7100
      IF(NL.EQ.2) GO TO 7200
C
C************** G,P,T,W, OF STEADY STATE ******************************
C
 7100 CONTINUE
      DO 200 LL=1,J
      CALL MOMENT ( 1 )
      CALL TEMPRT ( 1 )
      CALL GASPEC ( 1 )
C
      EPS=0.0
      DO 210 I=1,M
      IF (DABS((GA2(I)-GG(I))/GA2(I)).GT.EPS)  EPS=DABS((GA2(I)
     *-GG(I))/GA2(I))
      IF (DABS((TO2(I)-TTO(I))/TO2(I)).GT.EPS)  EPS=DABS((TO2(I)
     *-TTO(I))/TO2(I))
 210  CONTINUE
      DO 220 I=1,N
      IF (DABS((TN2(I)-TTN(I))/TN2(I)).GT.EPS)  EPS=
     *DABS((TN2(I)-TTN(I))/TN2(I))
 220  CONTINUE
      DO 230 I=1,N
      DO 230 JJ=1,K
      IF (DABS(WN2(I,JJ)-WWN(I,JJ)).GT.EPS) EPS=DABS(WN2(
     *I,JJ)-WWN(I,JJ))
 230  CONTINUE
      DO 235 I=1,M
      DO 235 JJ=1,K
      IF (DABS(WO2(I,JJ)-WWO(I,JJ)).GT.EPS) EPS=DABS(WO2(I,JJ)
     *-WWO(I,JJ))
 235  CONTINUE
C
      IF (EPS.LE.1.0E-3) GO TO 400
C
      DO 250 I=1,M
      GA1(I)=0.7*GG(I)+0.3*GA2(I)
      GG(I)=GA1(I)
      TO1(I)=0.7*TTO(I)+0.3*TO2(I)
      TA1(I)=0.7*TTA(I)+0.3*TA2(I)
      TTO(I)=TO1(I)
      TTA(I)=TA1(I)
 250  CONTINUE
      DO 260 I=1,N
      TN1(I)=0.7*TTN(I)+0.3*TN2(I)
      TTN(I)=TN1(I)
 260  CONTINUE
      DO 280 I=1,N
```

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      DO 280 JJ=1,K
      WN1(I,JJ)=0.7*WWN(I,JJ)+0.3*WN2(I,JJ)
      WWN(I,JJ)=WN1(I,JJ)
  280 CONTINUE
      DO 290 I=1,M
      DO 290 JJ=1,K
      WO1(I,JJ)=0.7*WWO(I,JJ)+0.3*WO2(I,JJ)
      WWO(I,JJ)=WO1(I,JJ)
      WA1(I,JJ)=0.7*WAA(I,JJ)+0.3*WA2(I,JJ)
      WAA(I,JJ)=WA1(I,JJ)
  290 CONTINUE
      DO 292 JJ=1,K
      SCH(JJ)=SC(5,JJ)
  292 OMGB(JJ) = WA2(5,JJ)
      CALL BNDCHM ( RE(5), SCH, H(5)/D(5), D(5), C(3), C(13),
     1              DEA1(5)/C(3), OMGB, TWA(5), PA2(5), AVEMOL(5),
     2              OMGW, GM1(5) )
      DO 294 JJ=1,K
      WWA(5,JJ) = OMGW(JJ)
      SCH(JJ)=SC(11,JJ)
  294 OMGB(JJ) = WA2(11,JJ)
      CALL BNDCHM ( RE(11), SCH, H(11)/D(11), D(11), C(3), C(13),
     1              DEA1(11)/C(3), OMGB, TWA(11), PA2(11), AVEMOL(11),
     2              OMGW, GM1(11) )
      DO 298 JJ=1,K
  298 WWA(11,JJ) = OMGW(JJ)
      DO 240 I=1,M
        IF ( I.EQ.5.OR.I.EQ.11 )   GO TO 240
      DO 245 JJ=1,K
  245 WWA(I,JJ) = WA2(I,JJ)
  240 CONTINUE
C
      CALL PROPER
  200 CONTINUE
C
        WRITE(6,*) '*****  ITERATION TIME IS OVER AT STEADY STATE !!
     1          ,'  *****'
C
  400 WRITE(6,3020) LL
      WRITE(6,3100) (I,P2(I),I=1,N)
      WRITE(6,3110) (I,GA2(I),I=1,M)
      WRITE(6,3120) (I,RE(I),I=1,M)
      WRITE(6,3130) (I,TN2(I),I=1,N)
      WRITE(6,3145) (I,TA2(I),I=1,M)
      WRITE(6,3140) (I,TO2(I),I=1,M)
      DO 405 KPRT=2,5
      WRITE(6,3150) KPRT, (I,WN2(I,KPRT),I=1,N)
      WRITE(6,3180)       (I,WA2(I,KPRT),I=1,M)
      WRITE(6,3160)       (I,WO2(I,KPRT),I=1,M)
  405 WRITE(6,3170)       (I,WWA(I,KPRT),I=1,M)
      STOP
C
C******************* G, P, T, W OF TRANSIENT STATE *******************
C
 7200 ND=INT(TIME/DTI)
      ETIME = 0.0
      DT    = DTI
C
      DO 1000 KK=1,ND
      EPST=0.0
```

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00000176        ETIME=ETIME+DT
            C
00000177        DO 500 L=1,J
            C
00000178        CALL MOMENT ( NSORT )
00000179        CALL TEMPRT ( 1 )
00000180        CALL GASPEC ( 1 )
            C
00000181        EPS=0.0
00000182        DO 510 I=1,M
00000183        IF (DABS((GA2(I)-GG(I))/GG(I)).GT.EPS) EPS=DABS((GA2(I)-GG(I))/
               *    GG(I))
00000184        IF (DABS((TO2(I)-TTO(I))/TTO(I)).GT.EPS) EPS=DABS((TO2(I)-TTO(I))
               */TTO(I))
00000185 510    CONTINUE
00000186        DO 520 I=1,N
00000187        IF (DABS((TN2(I)-TTN(I))/TTN(I)).GT.EPS) EPS=DABS((TN2(I)-TTN(I))
               */TTN(I))
00000188 520    CONTINUE
00000189        DO 530 I=1,N
00000190        DO 530 JJ=1,K
00000191        IF (DABS(WN2(I,JJ)-WWN(I,JJ)).GT.EPS) EPS=DABS(WN2(I,JJ)
               *-WWN(I,JJ))
00000192 530    CONTINUE
00000193        DO 540 I=1,M
00000194        DO 540 JJ=1,K
00000195        IF(DABS(WO2(I,JJ)-WWO(I,JJ)).GT.EPS) EPS=DABS(WO2(I,JJ)
               *-WWO(I,JJ))
00000196 540    CONTINUE
            C
            C-----    JUDGEMENT OF CONVERGENCE    -----
            C
00000197        IF (EPS.LE.1.0E-3) GO TO 300
00000198        DO 650 I=1,M
00000199        GA1(I)=0.7*GG(I)+0.3*GA2(I)
00000200        GG(I)=GA1(I)
00000201        TO1(I)=0.7*TTO(I)+0.3*TO2(I)
00000202        TA1(I)=0.7*TTA(I)+0.3*TA2(I)
00000203        TTO(I)=TO1(I)
00000204        TTA(I)=TA1(I)
00000205 650    CONTINUE
00000206        DO 660 I=1,N
00000207        TN1(I)=0.7*TTN(I)+0.3*TN2(I)
00000208        TTN(I)=TN1(I)
00000209 660    CONTINUE
00000210        DO 680 I=1,N
00000211        DO 680 JJ=1,K
00000212        WN1(I,JJ)=0.7*WWN(I,JJ)+0.3*WN2(I,JJ)
00000213        WWN(I,JJ)=WN1(I,JJ)
00000214 680    CONTINUE
00000215        DO 690 I=1,M
00000216        DO 690 JJ=1,K
00000217        WO1(I,JJ)=0.7*WWO(I,JJ)+0.3*WO2(I,JJ)
00000218        WWO(I,JJ)=WO1(I,JJ)
00000219        WA1(I,JJ)=0.7*WAA(I,JJ)+0.3*WA2(I,JJ)
00000220        WAA(I,JJ)=WA1(I,JJ)
00000221 690    CONTINUE
00000222        DO 692 JJ=1,K
00000223        SCH(JJ)=SC(5,JJ)
00000224 692    OMGB(JJ) = WA2(5,JJ)
```

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00000225          CALL BNDCHM ( RE(5), SCH, H(5)/D(5), D(5), C(3), C(13),
                 1              DEA1(5)/C(3), OMGB, TWA(5), PA2(5), AVEMOL(5),
                 2              OMGW, GM1(5) )
00000226          DO 694 JJ=1,K
00000227          WWA(5,JJ) = OMGW(JJ)
00000228          SCH(JJ)=SC(11,JJ)
00000229 694      OMGB(JJ) = WA2(11,JJ)
00000230          CALL BNDCHM ( RE(11), SCH, H(11)/D(11), D(11), C(3), C(13),
                 1              DEA1(11)/C(3), OMGB, TWA(11), PA2(11), AVEMOL(11),
                 2              OMGW, GM1(11) )
00000231          DO 698 JJ=1,K
00000232 698      WWA(11,JJ) = OMGW(JJ)
00000233          DO 640 I=1,M
00000234            IF ( I.EQ.5.OR.I.EQ.11 )    GO TO 640
00000235          DO 645 JJ=1,K
00000236 645      WWA(I,JJ) = WA2(I,JJ)
00000237 640      CONTINUE
00000238          CALL PROPER
00000239 500      CONTINUE
         C
00000240            WRITE(6,*) '*****  ITERATION TIME IS OVER AT TRANSIENT STATE !!'
                 1          ,'   *****'
         C
00000241 300      WRITE(6,3000) ETIME, KK
00000242          WRITE(6,3100) (I,P2(I),I=1,N)
00000243          WRITE(6,3110) (I,GA2(I),I=1,M)
00000244          WRITE(6,3120) (I,RE(I),I=1,M)
00000245          WRITE(6,3130) (I,TN2(I),I=1,N)
00000246          WRITE(6,3145) (I,TA2(I),I=1,M)
00000247          WRITE(6,3140) (I,TO2(I),I=1,M)
00000248          DO 415 KPRT=2,5
00000249          WRITE(6,3150) KPRT, (I,WN2(I,KPRT),I=1,N)
00000250          WRITE(6,3180)       (I,WA2(I,KPRT),I=1,M)
00000251          WRITE(6,3160)       (I,WO2(I,KPRT),I=1,M)
00000252 415      WRITE(6,3170)       (I,WWA(I,KPRT),I=1,M)
         C
00000253          DO 800 I=1,M
00000254          IF (DABS((GA2(I)-GGT(I))/GGT(I)).GT.EPST) EPST=DABS((GA2(I)
                 *-GGT(I))/GGT(I))
00000255          IF (DABS((TO2(I)-TTOT(I))/TTOT(I)).GT.EPST) EPST=DABS((TO2(I)
                 *-TTOT(I))/TTOT(I))
00000256          DO 800 JJ=1,K
00000257          IF(DABS(WO2(I,JJ)-WWOT(I,JJ)).GT.EPST) EPST=DABS(WO2(I,JJ)
                 *-WWOT(I,JJ))
00000258 800      CONTINUE
00000259          DO 810 I=1,N
00000260          IF (DABS((TN2(I)-TTNT(I))/TTNT(I)).GT.EPST) EPST=DABS((TN2(I)
                 *-TTNT(I))/TTNT(I))
00000261          DO 810 JJ=1,K
00000262          IF (DABS(WN2(I,JJ)-WWNT(I,JJ)).GT.EPST) EPST=DABS(WN2(I,JJ)
                 *-WWNT(I,JJ))
00000263 810      CONTINUE
         C
00000264          IF (EPST.LE.1.0E-5) GO TO 2000
         C
00000265          DO 900 I=1,M
00000266          GGT(I)=GA2(I)
00000267          TTOT(I)=TO2(I)
00000268          TTAT(I)=TA2(I)
00000269          DO 900 JJ=1,K
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      WWOT(I,JJ)=WO2(I,JJ)
      WAAT(I,JJ)=WA2(I,JJ)
  900 CONTINUE
      DO 910 I=1,N
      DO 910 JJ=1,K
      TTNT(I)=TTN(I)
      WWNT(I,JJ)=WWN(I,JJ)
  910 CONTINUE
C
      CALL PROPER
C
 1000 CONTINUE
      STOP
C
 2000 WRITE(6,3010) ETIME, KK
      WRITE(6,3100) (I,P2(I),I=1,N)
      WRITE(6,3110) (I,GA2(I),I=1,M)
      WRITE(6,3120) (I,RE(I),I=1,M)
      WRITE(6,3130) (I,TN2(I),I=1,N)
      WRITE(6,3145) (I,TA2(I),I=1,M)
      WRITE(6,3140) (I,TO2(I),I=1,M)
      DO 425 KPRT=2,5
      WRITE(6,3150) KPRT, (I,WN2(I,KPRT),I=1,N)
      WRITE(6,3180)       (I,WA2(I,KPRT),I=1,M)
      WRITE(6,3160)       (I,WO2(I,KPRT),I=1,M)
  425 WRITE(6,3170)       (I,WWA(I,KPRT),I=1,M)
C
 3000 FORMAT(1H0,//,'    *****   TIME =',F8.3,' (SEC)   ITER.NO.=',
     *        I3,'   *****' )
 3010 FORMAT(1H1,/,20('*'),'   STEADY STATE IN TRANSIENT CALCULATION',
     *     '   TIME = ',F8.3,' (SEC)   ITER.NO.=',I3,'    ',20('*'))
 3020 FORMAT(1H1,/,20('*'),'   STEADY STATE !!',
     *     '      LL = ',I3,'     ',60('*'))
 3100 FORMAT(1H0,'  <PRESSURE AT NODE>',        /,1X,8(I2,1PE14.7,1X),/,
     *  1X,8(I2,E14.7,1X),/,1X,8(I2,E14.7,1X),/,1X,8(I2,E14.7,1X))
 3110 FORMAT(1H0,'  <FLOW RATE OF BRANCH>',    /,1X,8(I2,1PE13.5,2X),/,
     *  1X,8(I2,E13.5,2X),/,1X,8(I2,E13.5,2X),/,1X,8(I2,E13.5,2X))
 3120 FORMAT(1H ,'  <REYNOLDS NUMBER>',         /,1X,10(I2,F8.2,3X),/,
     *  1X,10(I2,F8.2,3X),/,1X,10(I2,F8.2,3X))
 3130 FORMAT(1H0,'  <TEMPERATURE AT NODE>',     /,1X,10(I2,F8.2,3X),/,
     *  1X,10(I2,F8.2,3X),/,1X,10(I2,F8.2,3X))
 3135 FORMAT(1H ,'  <TEMPERATURE AT WALL>',     /,1X,10(I2,F8.2,3X),/,
     *  1X,10(I2,F8.2,3X),/,1X,10(I2,F8.2,3X))
 3140 FORMAT(1H ,'  <TEMP. OF BRANCH OUTLET>',/,1X,10(I2,F8.2,3X),/,
     *  1X,10(I2,F8.2,3X),/,1X,10(I2,F8.2,3X))
 3145 FORMAT(1H ,'  <AVERAGE TEMP. OF BRANCH>',/,1X,10(I2,F8.2,3X),/,
     *  1X,10(I2,F8.2,3X),/,1X,10(I2,F8.2,3X))
 3150 FORMAT(1H0,'  <CONCENTRATION AT NODE>  GAS =',I2,' : 1=HE, 2=O2',
     *           ', 3=CO, 4=CO2, 5=N2 ---',/,
     *  1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X))
 3160 FORMAT(1H ,'  <CONC. OF BRANCH OUTLET>  ',/,
     *  1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X))
 3170 FORMAT(1H ,'  <CONCENTRATION ON WALL>  ',/,
     *  1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X))
 3180 FORMAT(1H ,'  <AVERAGE CONCENTRATION OF BRANCH>',/,
     *  1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X),/,1X,10(I2,F9.5,2X))
      STOP
      END
```

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         C
         C**********************************************************************
         C*****                                                            *****
         C*****         TO CALCULATE MASS FLOW RATE AND PRESSURE           *****
         C*****                                                            *****
00000001                    SUBROUTINE MOMENT  ( KK )
         C*****                                                            *****
         C**********************************************************************
         C
00000002       IMPLICIT REAL*8 (A-H,O-Z)
00000003       PARAMETER (N=26, M=27, K=5, J=200, PI=3.141592645, GRAV=9.807 )
00000004       DIMENSION H(M),D(M),Y(M),F(M),TA1(M),GA1(M),GA2(M),PA1(M),PA2(M),
              *PN1(N),PN2(N),DEA1(M),DI(M,K),CP(M),RE(M),GR(M),PR(M),
              *SC(M,K),SH(M,K),C(13),AG(M),BG(M),AAG(M,M+1),P1(N),GA(M),
              *WA1(M,K),DEO(M),DEI(M),TN1(N),TI1(M),TI2(M),P2(N),GM1(M),
              *TO1(M),TO2(M),TA2(M),WI1(M,K),WI2(M,K),WO1(M,K),WO2(M,K),TN2(N),
              *WA2(M,K),S(M,M),CAT(M),Q(M),
              *GX1(M),GX2(M),PX1(N),PX2(M),TWA(M),CPN(M),CPO(M),
              *AVEMOL(M),WN1(N,K),WN2(N,K),WWA(M,K),
              *TTAT(M),GGT(M),WAAT(M,K),PP(N),PPT(N),PAT(M),CPT(M),DEAT(M)
00000005       REAL*8 NNI(M),NNO(M),MU(M),LAM(M),NU(M),MOLW(K+1)
         C
00000006       COMMON/SIZE/H,D,Y,F,NNI,NNO,CAT,DT
              *       /TEMP/TI1,TI2,TO1,TO2,TA1,TA2,TN1,TN2,TWA,TTAT
              *       /PRES/P1,P2,PN1,PN2,PA1,PA2,PP,PPT,PAT
              *       /COMP/WI1,WI2,WO1,WO2,WA1,WA2,WN1,WN2,WAAT,WWA
              *       /FLOW/GA1,GA2,GA,GGT,GM1
              *       /QUAL/DI,CP,CPT,CPO,CPN,MU,LAM,DEI,DEO,DEA1,DEAT
              *       /MLWG/MOLW,AVEMOL,C
              *       /REFE/RE,GR,PR,NU,SC,SH,Q
         C
00000007       DO 200  L=1,J
00000008       DO 30 I=1,M
00000009       AG(I) = 0.0
00000010       BG(I) = 0.0
00000011       DO 30 JJ=1,M+1
00000012       AAG(I,JJ)=0.0
00000013 30    CONTINUE
00000014       DO  80 I=1,M
00000015       PX1(NNI(I))=(P1(NNI(I))-C(1))*D(I)**2/C(3)/C(13)**2
00000016       IF(I.EQ.1) THEN
00000017       PX1(NNI(I))=0.0
00000018       END IF
00000019       IF(I.EQ.M) THEN
00000020       PX1(NNO(I))=0.0
00000021       END IF
00000022       PA1(I)=(P1(NNI(I))+P1(NNO(I)))/2.0
00000023 80    CONTINUE
         C
         C***************** COEFFICIENTS OF MATRIX ******************************
         C
00000024       DO 150 I=1,M
00000025       GX1(I)=GA1(I)*D(I)/C(3)/C(13)
00000026       RE(I)=DABS(GA1(I)*D(I)/MU(I))
00000027       F(I) = FRIC ( RE(I),H(I)/D(I) )
00000028       GR(I)=(C(3)-C(4))*GRAV*D(I)**3/C(3)/C(13)**2
00000029       IF (KK.EQ.1) THEN
00000030       AG(I)=AG(I)+(4.0*F(I)+D(I)/H(I)*Y(I))*DABS(GX1(I))/2./DEA1(I)
              **C(3)*H(I)/D(I)
00000031       AG(I)=AG(I)*C(3)*C(13)**2/D(I)**2
```

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      BG(I)=BG(I)+GX1(I)*DABS(GX1(I))*(C(3)/DEO(I)-C(3)/DEI(I))
      BG(I)=BG(I)+GR(I)*(DEA1(I)-C(3))/(C(3)-C(4))*H(I)*
     *DCOS(PI/180.0*CAT(I))/D(I)
      BG(I)=BG(I)*C(3)*C(13)**2/D(I)**2
      END IF
      IF(KK.EQ.2) THEN
      AG(I)=AG(I)+(4.0*F(I)+D(I)/H(I)*Y(I))*DABS(GX1(I))/2./DEA1(I)
     **C(3)*H(I)/D(I)
      AG(I)=AG(I)+H(I)*D(I)/DT/C(13)
      AG(I)=AG(I)*C(3)*C(13)**2/D(I)**2
      BG(I)=BG(I)+GX1(I)*DABS(GX1(I))*(C(3)/DEO(I)-
     *C(3)/DEI(I))
      BG(I)=BG(I)+GR(I)*(DEA1(I)-C(3))/(C(3)-C(4))*H(I)*
     *DCOS(PI/180.0*CAT(I))/D(I)
      BG(I)=BG(I)-GGT(I)*D(I)/C(3)/C(13)*H(I)*D(I)/DT/C(13)
      BG(I)=BG(I)*C(3)*C(13)**2/D(I)**2
      END IF
  130 CONTINUE
  150 CONTINUE
C
C*********** INPUT THE COEFFICIENTS OF THE MATRIX *********************
C
      DO 100 I=1,M
      DO 100 JJ=1,M
      S(I,JJ)=PI/4.0*D(JJ)*C(3)*C(13)
  100 CONTINUE
      AAG(1,1)=S(1,1)
      AAG(1,2)=-S(1,2)
      AAG(1,8)=-S(1,8)
      AAG(1,14)=-S(1,14)
      DO 500 I=2,6
      AAG(I,I)=S(I,I)
      AAG(I,I+1)=-S(I,I+1)
  500 CONTINUE
      DO 510 I=8,12
      AAG(I,I)=S(I,I)
      AAG(I,I+1)=-S(I,I+1)
  510 CONTINUE
      AAG(7,7)=S(7,7)
      AAG(7,13)=S(7,13)
      AAG(7,19)=S(7,19)
      AAG(7,20)=-S(7,20)
      DO 520 I=2,7
      AAG(13,I)=-AG(I)
  520 CONTINUE
      DO 525 I=8,13
      AAG(13,I)=AG(I)
  525 CONTINUE
      DO 530 I=14,18
      AAG(I,I)=S(I,I)
      AAG(I,I+1)=-S(I,I+1)
  530 CONTINUE
      DO 540 I=8,13
      AAG(19,I)=-AG(I)
  540 CONTINUE
      DO 550 I=14,19
      AAG(19,I)=AG(I)
  550 CONTINUE
      DO 560 I=20,26
      AAG(I,I)=S(I,I)
```

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00000085          AAG(I,I+1)=-S(I,I+1)
00000086 560      CONTINUE
00000087          DO 570 I=14,27
00000088          AAG(27,1)=-AG(1)
00000089          AAG(27,I)=-AG(I)
00000090 570      CONTINUE
00000091          AAG(13,M+1)=BG(2)+BG(3)+BG(4)+BG(5)+BG(6)+BG(7)-BG(8)
                *-BG(9)-BG(10)-BG(11)-BG(12)-BG(13)
00000092          AAG(19,M+1)=BG(8)+BG(9)+BG(10)+BG(11)+BG(12)+BG(13)-BG(14)
                *-BG(15)-BG(16)-BG(17)-BG(18)-BG(19)
00000093          AAG(27,M+1)=BG(1)+BG(14)+BG(15)+BG(16)+BG(17)+BG(18)+BG(19)
                *+BG(20)+BG(21)+BG(22)+BG(23)+BG(24)+BG(25)+BG(26)+BG(27)
         C
00000094          DMLES5 = PI/4.0*D(5)**2*H(5)
00000095          DMLES1 = PI/4.0*D(11)**2*H(11)
00000096          IF (GX1(5).LT.0.0) THEN
00000097          AAG(4,M+1)=-GM1(5) * DMLES5
00000098          AAG(5,M+1)=0.0
00000099          ELSE IF (GX1(5).GE.0.0) THEN
00000100          AAG(4,M+1)=0.0
00000101          AAG(5,M+1)=-GM1(5) * DMLES5
00000102          END IF
00000103          IF (GX1(11).LT.0.0) THEN
00000104          AAG(10,M+1)=-GM1(11) * DMLES1
00000105          AAG(11,M+1)=0.0
00000106          ELSE IF (GX1(11).GE.0.0) THEN
00000107          AAG(10,M+1)=0.0
00000108          AAG(11,M+1)=-GM1(11) * DMLES1
00000109          END IF
         C
         C****************** TO SOLVE MATRIX *************************************
         C
00000110          CALL GAUELD (AAG,M,M,M+1,1.0E-10,ILL)
00000111          IF(ILL.EQ.0) GO TO 1
00000112          WRITE(6,*) 'GAUELD AT MOMENT ; L, ILL   ',L,ILL
00000113          STOP
00000114 1        JJ=M+1
00000115          DO 2 I=1,M
00000116          GA1(I)=AAG(I,JJ)*C(3)*C(13)/D(I)
00000117 2        CONTINUE
         C
         C************** JUDGEMENT OF CONVERGENCE *****************************
         C
00000118          EPS=1.0E-4
00000119          DO 50 I=1,M-1
00000120          IF (DABS((AAG(I+1,M+1)-GX1(I+1))/DABS(GX1(I+1))).GT.
                *DABS((AAG(I,M+1)-GX1(I))/DABS(GX1(I))))
                *TTA=DABS((AAG(I+1,M+1)-GX1(I+1))/GX1(I+1))
00000121 50       CONTINUE
00000122          IF (TTA.LE.EPS) GO TO 40
00000123          DO 210 JJ=1,M
00000124          GX1(JJ)=GX1(JJ)+0.3*(AAG(JJ,M+1)-GX1(JJ))
00000125          GA1(JJ)=GX1(JJ)*C(3)*C(13)/D(JJ)
00000126 210      CONTINUE
00000127 200      CONTINUE
00000128            WRITE(6,*) '*****  ITERATION TIME IS OVER AT MOMENT SUBROUTINE'
               1             ,' !!  *****'
         C
         C****************** CONVERGED!!!!***************************************
         C
```

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```
 40     DO 60 I=1,M
        GX2(I)=AAG(I,M+1)
        GA2(I)=GX2(I)*C(3)*C(13)/D(I)
          IF ( ABS(GA2(I)).LT.1.0E-6 )      GA2(I)=1.0E-6
        PX2(1)=0.0
        P2(1)=1.0E+5
        P2(NNO(I))=P2(NNI(I))-AG(I)*GX2(I)-BG(I)
        PX2(NNO(I))=(P2(NNO(I))-C(1))*D(I)**2/C(3)/C(13)**2
 60     CONTINUE
        DO 65 I=1,M
        PA2(I)=(P2(NNI(I))+P2(NNO(I)))/2.0
 65     CONTINUE
        DO 90 I=1,M
        PX1(NNI(I))=PX2(NNI(I))
        PX1(NNI(I))=PX2(NNO(I))
        P1(NNI(I))=P2(NNI(I))
        P1(NNO(I))=P2(NNO(I))
        PA1(I)=PA2(I)
        GX1(I)=GX2(I)
        GA1(I)=GA2(I)
 90     CONTINUE
        RETURN
        END
```

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         C
         C************************************************************************
         C*****                                                              *****
         C*****                    THERMAL PROPERTIES OF GAS                 *****
         C*****                                                              *****
00000001                           SUBROUTINE PROPER
         C*****                                                              *****
         C************************************************************************
         C
         C      DI   ; DIFFUSION FACTOR IN MIXTURE GAS          (M**2/S)
         C      CP   ; SPECIFIC HEAT OF MIXTURE GAS             (J/KG.K)
         C      MU   ; VISCOSITY OF MIXTURE GAS                 (PA.S)
         C      LAM  ; THERMAL CONDUCTIVITY OF MIXTURE GAS      (W/M.K)
         C      DEA1 ; DENSITY OF MIXTURE GAS                   (KG/M**3)
         C      T    ; TEMPRETURE OF MIXTURE GAS (K)
         C      PP   ; PRESSURE OF MIXTURE GAS (PA)
         C
00000002        IMPLICIT REAL*8 (A-H,O-Z)
00000003        PARAMETER (N=26, M=27, K=5)
00000004        DIMENSION H(M),D(M),Y(M),F(M),NNI(M),NNO(M),CP(M),
               1          W2(K),W3(K),W4(K),W5(K),GA1(M),GA2(M),WN1(N,K),
               2          CPOT(M),CPN(M),CPT(M),DEAT(M),AVEMOL(M),WN2(N,K),
               * W(K),DIM(K),DDI(K,K),P1(N),P2(N),PN2(N),PP1(M),PPT(M),PAT(M),
               * AMU(6), AD(8), TD(K,K), OMIKAD(K,K), FIB(K,K), FIA(K,K),EA(K),
               *RA(K),CCP(K), CPA(K,4), TMU(K), OMIKAV(K),  CPO(K), WFIA(K),
               *TI1(M),TI2(M),TO1(M),TO2(M),TA1(M),TA2(M),TN1(N),PN1(N),
               *PA1(M),PA2(M),WI1(M,K),WI2(M,K),WO1(M,K),WO2(M,K),WA1(M,K),
               *WA2(M,K),DI(M,K),DEI(M),DEO(M),DEA1(M),WAAT(M,K),WWA(M,K),
               *CPA1(K),TN2(N),TWA(M), TTAT(M)
00000005        REAL*8 LAS(K), MUS(K), LA(K), MU(M), LAM(M), MOLW(K+1), MUM,
               *         NNI, NNO, LAMM
00000006        COMMON/TEMP/TI1,TI2,TO1,TO2,TA1,TA2,TN1,TN2, TWA, TTAT
               */PRES/P1, P2, PN1, PN2, PA1, PA2, PP1, PPT, PAT
               */COMP/WI1,WI2,WO1,WO2,WA1,WA2,WN1,WN2,WAAT, WWA
               */QUAL/DI,CP,CPT,CPOT,CPN,MU,LAM,DEI,DEO,DEA1,DEAT
               */MLWG/MOLW,AVEMOL
               */FLOW/GA1,GA2
               */SIZE/H,D,Y,F,NNI,NNO
         C
00000007        DATA AD/1.06036, 0.15610, 0.19300, 0.47635, 1.03587, 1.52996,
               *     1.76474, 3.89411/
               *     EA/10.22, 106.7, 91.7, 195.2, 71.4/
               *     RA/2.551, 3.467, 3.690, 3.941, 3.798/
               *     AMU/1.16145, 0.14874, 0.52487, 0.77320, 2.16178, 2.43787/
00000008        DATA CPA1/4.9677, 6.713, 7.373, 4.728, 7.440/
00000009        DATA CPA/4.9677, 0.817026, 0.929207, 0.618542, 0.938314,
               *        0.0, 3.87124E-4,  3.43656E-4, 9.43157E-4, 2.95732E-4,
               *        0.0, -1.41476E-7, -1.00711E-7, -3.9229E-7, -7.31507E-8,
               *     0.0, 1.99678E-11, 1.01493E-11, 5.44078E-11, 5.81796E-12/
         C
00000010        DO 1000 II=1,M
00000011          T  = TA1(II) + 273.15
00000012          T2 = TTAT(II) + 273.15
00000013          T4 = TO1(II) + 273.15
00000014            III = NNI(II)
00000015            IIO = NNO(II)
00000016              IF ( GA2(II).LT.0.0 ) THEN
00000017            III = NNO(II)
00000018            IIO = NNI(II)
00000019              ENDIF
```

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00000020          PP   = PA1(II)
00000021          PP2  = PAT(II)
00000022            IF ( II.GT.N.OR.III.GT.N )    GO TO 1010
00000023          T3   = TN1(II) + 273.15
00000024          T5   = TN1(III) + 273.15
00000025          PP3 = P1(II)
00000026          PP4 = P1(II)
00000027          PP5 = P1(II)
00000028 1010       CONTINUE
00000029          DO 1100 JJ=1,K
00000030            W(JJ)   = WA1(II,JJ)
00000031            W2(JJ) = WAAT(II,JJ)
00000032            W4(JJ) = WO1(II,JJ)
00000033              IF ( II.GT.N )     GO TO 1100
00000034            W3(JJ) = WN1(II,JJ)
00000035            W5(JJ) = WN1(II,JJ)
00000036 1100     CONTINUE
         C
         C**************** DIFFUSION FACTOR IN MIXTURE GAS DIM(I) **************
         C
00000037        DO 140 I=1,K
00000038        DIM(I)=0.0
00000039 140    CONTINUE
00000040        DO 120 I=1,K
00000041        DO 120 JJ=1,K
00000042        IF(T.LE.0.0) THEN
00000043        TD(I,JJ)=273.15/(EA(I)*EA(JJ))**0.5
00000044        END IF
00000045        IF (T.GT.0.0) THEN
00000046        TD(I,JJ)=T/(EA(I)*EA(JJ))**0.5
00000047        END IF
00000048        OMIKAD(I,JJ)=AD(1)/TD(I,JJ)**AD(2)+AD(3)*DEXP(-AD(4)*TD(I,JJ))
               *+AD(5)*DEXP(-AD(6)*TD(I,JJ))
00000049        DDI(I,JJ)=1.858E-7*T**1.5*((MOLW(I)+MOLW(JJ))*1.0E+3)**0.5/
               *(MOLW(I)*1.0E+3)**0.5/(MOLW(JJ)*1.0E+3)**0.5/PP*0.98692E+5
               */OMIKAD(I,JJ)/((RA(I)+RA(JJ))/2.)**2
00000050        DIM(I)=DIM(I)+W(JJ)/DDI(I,JJ)
00000051 120    CONTINUE
00000052        DO 130 I=1,K
00000053        DIM(I)=1.0/DIM(I)
00000054 130    CONTINUE
         C
         C******************* SPECIFIC HEAT OF MIXTURE GAS ; CPM ***************
         C
00000055        CPM=0.0
00000056        DO 210 I=1,K
00000057        CCP(I)=(CPA(I,1)+CPA(I,2)*T+CPA(I,3)*T**2+CPA(I,4)*T**3)*1.0E+3
00000058        CPM=CPM+CCP(I)*W(I)
00000059 210    CONTINUE
00000060        CPM2=0.0
00000061        DO 220 I=1,K
00000062        CCP(I)=(CPA(I,1)+CPA(I,2)*T2+CPA(I,3)*T2**2+CPA(I,4)*T2**3)*1.0E+3
00000063        CPM2=CPM2+CCP(I)*W2(I)
00000064 220    CONTINUE
00000065        CPM4=0.0
00000066        DO 230 I=1,K
00000067        CCP(I)=(CPA(I,1)+CPA(I,2)*T4+CPA(I,3)*T4**2+CPA(I,4)*T4**3)*1.0E+3
00000068        CPM4=CPM4+CCP(I)*W4(I)
00000069 230    CONTINUE
00000070        CPM5=0.0
```

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00000071         DO 240 I=1,K
00000072         CCP(I)=(CPA(I,1)+CPA(I,2)*T5+CPA(I,3)*T5**2+CPA(I,4)*T5**3)*1.0E+3
00000073         CPM5=CPM5+CCP(I)*W5(I)
00000074 240     CONTINUE
         C
         C****************** VISCOSITY OF MIXTURE GAS ; MUM *******************
         C
00000075         MUM=0.0
00000076         DO 310 I=1,K
00000077         IF(T.LE.0.0) THEN
00000078         TMU(I)=273.15/EA(I)
00000079         END IF
00000080         IF(T.GT.0.0) THEN
00000081         TMU(I)=T/EA(I)
00000082         END IF
00000083         OMIKAV(I)=AMU(1)/TMU(I)**AMU(2)+AMU(3)*DEXP(-AMU(4)*TMU(I))
                *+AMU(5)*DEXP(-AMU(6)*TMU(I))
00000084         MUS(I)=26.69*(MOLW(I)*1.0E+3*T)**0.5*1.0E-7/OMIKAV(I)/RA(I)**2
00000085         WFIA(I)=0.0
00000086 310     CONTINUE
00000087         DO 320 I=1,K
00000088         DO 330 JJ=1,K
00000089         FIA(I,JJ)=(1.0+(MUS(I)/MUS(JJ))**0.5*(MOLW(JJ)/MOLW(I))
                ***0.25)**2/(8.0*(1.0+MOLW(I)/MOLW(JJ)))**0.5
00000090         WFIA(I)=WFIA(I)+W(JJ)*FIA(I,JJ)
00000091 330     CONTINUE
00000092         MUM=MUM+W(I)*MUS(I)/WFIA(I)
00000093 320     CONTINUE
         C
         C****************** THERMAL CONDUCTIVITY OF MIXTURE GAS ; LAMM ****
         C
00000094         LAMM=0.0
00000095         DO 410 I=1,K
00000096         LAS(I)=0.0
00000097         CPO(I)=CPA1(I)-1.986
00000098         LA(I)=4.186*(1.32*CPO(I)+3.52)*MUS(I)/MOLW(I)
00000099 410     CONTINUE
00000100         DO 430 I=1,K
00000101         DO 420 JJ=1,K
00000102         FIB(I,JJ)=(1.0+(LA(I)/LA(JJ))**0.5*(MOLW(JJ)/MOLW(I))**0.25)
                ***2/(8.0*(1.0+MOLW(I)/MOLW(JJ)))**0.5
00000103         LAS(I)=LAS(I)+W(JJ)*FIB(I,JJ)
00000104 420     CONTINUE
00000105         LAMM=LAMM+W(I)*LA(I)/LAS(I)
00000106 430     CONTINUE
         C
         C******************** DENSITY OF MIXTURE GAS ; DEM *******************
         C
00000107         AVEM  = 0.0
00000108         DO 510 I=1,K
00000109 510     AVEM  = AVEM  + W(I) /MOLW(I)
00000110         AVEM  = 1.0/AVEM
00000111         DEM   = AVEM *PP /8.314/T
00000112         AVEM2 = 0.0
00000113         DO 520 I=1,K
00000114 520     AVEM2 = AVEM2 + W2(I)/MOLW(I)
00000115         AVEM2 = 1.0/AVEM2
00000116         DEM2  = AVEM2*PP2/8.314/T2
00000117         AVEM3 = 0.0
00000118         DO 530 I=1,K
```

```
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 530   AVEM3 = AVEM3 + W3(I)/MOLW(I)
       AVEM3 = 1.0/AVEM3
       DEM3  = AVEM3*PP3/8.314/T3
       AVEM4 = 0.0
       DO 540 I=1,K
 540   AVEM4 = AVEM4 + W4(I)/MOLW(I)
       AVEM4 = 1.0/AVEM4
       DEM4  = AVEM4*PP4/8.314/T4
C
C****************   REPLACEMENT OF EACH THERMAL PROPERTIES   **********
C
       DO 1200 JJ=1,K
 1200    DI(II,JJ) = DIM(JJ)
       CP(II)    = CPM
       CPT(II)   = CPM2
       CPOT(II)  = CPM4
       CPN(II)   = CPM5
       MU(II)    = MUM
       LAM(II)   = LAMM
       AVEMOL(II) = AVEM
       DEA1(II) = DEM
       DEAT(II) = DEM2
       DEI(II)  = DEM3
       DEO(II)  = DEM4
         IF ( GA2(II).LT.0.0 )  THEN
       DEI(II)  = DEM4
       DEO(II)  = DEM3
         ENDIF
C
 1000  CONTINUE
C
       RETURN
       END
```

```
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              C
              C*************************************************************************
              C*****                                                                *****
              C*****        TO SOLVE TEMPERATURE OF NODE AND BRANCH OUTLET          *****
              C*****                                                                *****
00000001                        SUBROUTINE  TEMPRT  ( KK )
              C*****                                                                *****
              C*************************************************************************
              C
00000002            IMPLICIT REAL*8 (A-H,O-Z)
00000003            PARAMETER (N=26, M=27, K=5, J=200, PI=3.14159264 )
              C
00000004            DIMENSION H(M),D(M),Y(M),F(M),CAT(M),
                   *TI1(M),TI2(M),TO1(M),TO2(M),TA1(M),TA2(M),TN1(N),TN2(N),TWA(M),
                   *TTAT(M),
                   *P1(N),P2(N),PN1(N),PN2(N),PA1(M),PA2(M),PP(N),PPT(N),PAT(M),
                   *GA1(M),GA2(M),GA(M),GGT(M),
                   *DI(M,K),CP(M),DEI(M),DEO(M),DEA1(M),
                   *CPN(M),CPO(M),CPT(M),DEAT(M),NI(M),NO(M),
                   *RE(M),GR(M),PR(M),SC(M,K),SH(M,K),Q(M),
                   *AAT(2*M-1,2*M),CS(2*M),TA(2*M-1),
                   *WI1(M,K),WI2(M,K),WO1(M,K),WO2(M,K),WA1(M,K),WA2(M,K),
                   *WN1(N,K),WN2(N,K),WAAT(M,K),AVEMOL(M),C(13),
                   *AT(M),CT(M),DDT(M),ET(M),ST(2*M),BT(M),GX2(M),TX1(N+M)
00000005            REAL*8 NNI(M),NNO(M),MU(M),LAM(M),NU(M),MOLW(K+1)
              C
00000006            COMMON/SIZE/H,D,Y,F,NNI,NNO,CAT,DT
                   *    /TEMP/TI1,TI2,TO1,TO2,TA1,TA2,TN1,TN2,TWA,TTAT
                   *    /PRES/P1,P2,PN1,PN2,PA1,PA2,PP,PPT,PAT
                   *    /COMP/WI1,WI2,WO1,WO2,WA1,WA2,WN1,WN2,WAAT
                   *    /FLOW/GA1,GA2,GA,GGT
                   *    /QUAL/DI,CP,CPT,CPO,CPN,MU,LAM,DEI,DEO,DEA1,DEAT
                   *    /MLWG/MOLW,AVEMOL,C
                   *    /REFE/RE,GR,PR,NU,SC,SH,Q
              C
00000007            DO 200 L=1,J
00000008            DO 30 JJ=1,2*M-1
00000009            DO 30 KJ=1,2*M
00000010            AAT(JJ,KJ)=0.0
00000011 30         CONTINUE
00000012            DO 150 I=1,M
00000013            AT(I) = 0.0
00000014            BT(I) = 0.0
00000015            CT(I) = 0.0
00000016            DDT(I) = 0.0
00000017            ET(I)  = 0.0
00000018            IF (GA2(I)/DABS(GA2(I)).LT.0.0) THEN
00000019            NI(I)=NNO(I)
00000020            NO(I)=NNI(I)
00000021            END IF
00000022            IF (GA2(I)/DABS(GA2(I)).GE.0.0) THEN
00000023            NI(I)=NNI(I)
00000024            NO(I)=NNO(I)
00000025            END IF
00000026 150        CONTINUE
              C
              C************  HEAT TRANSFER AND OTHER COEFFICIENTS  *******************
              C
00000027            DO 350 I=1,M
00000028            PR(I)=MU(I)*CP(I)/LAM(I)
```

```
          FORTRAN77 EX    V12L10    TEMPRT       DATE 92-09-21   TIME 20:42:03

00000029        NU(I) = HTC ( RE(I), PR(I), H(I)/D(I) )
00000030        CT(I)=4.0*NU(I)*LAM(I)*H(I)/D(I)/C(13)/C(3)/C(7)
00000031        ET(I)=ET(I)+D(I)**2/C(2)/C(6)/C(13)*H(I)/D(I)*Q(I)
00000032        GX2(I)=GA2(I)*D(I)/C(3)/C(13)
             C
00000033        IF (KK.EQ.1) THEN
00000034        DDT(I)=CT(I)
00000035        AT(I)=CT(I)*(TWA(I)-TA1(I))/C(2) + ET(I)
00000036        ELSE
00000037        DDT(I)=CT(I)+DEA1(I)/C(3)*CP(I)/C(7)*H(I)*D(I)/DT/C(13)
00000038        ET(I)=ET(I)+DEAT(I)/C(3)*CPT(I)/C(7)*(TTAT(I)+273.15)/C(2)*
               *H(I)*D(I)/DT/C(13)
00000039        AT(I)=AT(I)+CT(I)*(TWA(I)+273.15)/C(2)
00000040        AT(I)=AT(I)-DDT(I)*(TA1(I)+273.15)/C(2)
00000041        AT(I)=AT(I)+ET(I)
00000042        END IF
00000043 350    CONTINUE
             C
             C***************** COEFFICIENTS OF MATRIX *****************************
             C
00000044        DO 100 I=1,M
00000045        ST(I)=PI/4.0*D(I)**2*DABS(GA2(I))*CPN(NI(I))*C(2)
00000046        IF(GA2(5)/DABS(GA2(5)).GE.0.0)
               *ST(5)=PI/4.0*D(5)**2*DABS(GA2(4))*CPN(NI(5))*C(2)
00000047        IF(GA2(5)/DABS(GA2(5)).LT.0.0)
               *ST(5)=PI/4.0*D(5)**2*DABS(GA2(6))*CPN(NI(5))*C(2)
00000048        IF(GA2(11)/DABS(GA2(11)).GE.0.0)
               *ST(11)=PI/4.0*D(11)**2*DABS(GA2(10))*CPN(NI(11))*C(2)
00000049        IF(GA2(11)/DABS(GA2(11)).LT.0.0)
               *ST(11)=PI/4.0*D(11)**2*DABS(GA2(12))*CPN(NI(11))*C(2)
00000050 100    CONTINUE
00000051        DO 120 I=M+1,2*M
00000052        ST(I)=-PI/4.0*D(I-M)**2*DABS(GA2(I-M))*CPO(I-M)*C(2)
00000053 120    CONTINUE
00000054        IF(GA2(1)/DABS(GA2(1)).LT.0.0) THEN
00000055        AAT(1,1)=1.0
00000056        AAT(1,M)=-1.0
00000057        END IF
00000058        IF(GA2(1)/DABS(GA2(1)).GE.0.0) THEN
00000059        AAT(1,1)=1.0
00000060        AAT(1,2*M)=1.0
00000061        END IF
00000062        IF(GA2(M)/DABS(GA2(M)).GE.0.0) THEN
00000063        AAT(N,N)=1.0
00000064        AAT(N,N+M)=-1.0
00000065        END IF
00000066        IF(GA2(M)/DABS(GA2(M)).LT.0.0) THEN
00000067        AAT(N,N)=1.0
00000068        AAT(N,2*M)=1.0
00000069        END IF
             C
00000070        DO 390 I=1,2*M
00000071        CS(I)=1.0
00000072 390    CONTINUE
00000073        DO 400 I=2,14,6
00000074        IF(GA2(I)/DABS(GA2(I)).GE.0.0) CS(I+M)=0.0
00000075        IF(GA2(I)/DABS(GA2(I)).LT.0.0) CS(I)=0.0
00000076        IF(GA2(1)/DABS(GA2(1)).GE.0.0) CS(1)=0.0
00000077        IF(GA2(1)/DABS(GA2(1)).LT.0.0) CS(M+1)=0.0
00000078        AAT(2,2)=CS(1)*ST(1)+CS(2)*ST(2)+CS(8)*ST(8)+CS(14)*ST(14)
```

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      AAT(2,I+N)=CS(I+M)*ST(I+M)
      AAT(2,M)=CS(M+1)*ST(M+1)
  400 CONTINUE
C
      DO 410 I=3,7
      IF(GA2(I)/DABS(GA2(I)).LT.0.0.OR.GA2(I-1)/DABS(GA2(I-1)).
     *LT.0.0) THEN
      AAT(I,I)=ST(I-1)
      AAT(I,I+N)=ST(I+M)
      GO TO 410
      END IF
      AAT(I,I)=ST(I)
      AAT(I,I+N-1)=ST(I+M-1)
  410 CONTINUE
C
      DO 420 I=8,12
      IF(GA2(I)/DABS(GA2(I)).LT.0.0.OR.GA2(I+1)/DABS(GA2(I+1)).
     *LT.0.0) THEN
      AAT(I,I)=ST(I)
      AAT(I,I+1+N)=ST(I+1+M)
      GO TO 420
      END IF
      AAT(I,I)=ST(I+1)
      AAT(I,I+N)=ST(I+M)
  420 CONTINUE
C
      DO 430 I=13,17
      IF(GA2(I+1)/DABS(GA2(I+1)).LT.0.0.OR.GA2(I+2)/DABS(GA2(I+2)).
     *LT.0.0) THEN
      AAT(I,I)=ST(I+1)
      AAT(I,I+2+N)=ST(I+2+M)
      GO TO 430
      END IF
      AAT(I,I)=ST(I+2)
      AAT(I,I+1+N)=ST(I+1+M)
  430 CONTINUE
C
      IF(GA2(7)/DABS(GA2(7)).GE.0.0) CS(7)=0.0
      IF(GA2(7)/DABS(GA2(7)).LT.0.0) CS(7+M)=0.0
      IF(GA2(13)/DABS(GA2(13)).GE.0.0) CS(13)=0.0
      IF(GA2(13)/DABS(GA2(13)).LT.0.0) CS(13+M)=0.0
      IF(GA2(19)/DABS(GA2(19)).GE.0.0) CS(19)=0.0
      IF(GA2(19)/DABS(GA2(19)).LT.0.0) CS(19+M)=0.0
      IF(GA2(20)/DABS(GA2(20)).GE.0.0) CS(20+M)=0.0
      IF(GA2(20)/DABS(GA2(20)).LT.0.0) CS(20)=0.0
      AAT(18,18)=CS(7)*ST(7)+CS(13)*ST(13)+CS(19)*ST(19)+CS(20)*ST(20)
      AAT(18,7+N)=CS(7+M)*ST(7+M)
      AAT(18,13+N)=CS(13+M)*ST(13+M)
      AAT(18,19+N)=CS(19+M)*ST(19+M)
      AAT(18,20+N)=CS(20+M)*ST(20+M)
C
      DO 440 I=19,25
      IF(GA2(I+1)/DABS(GA2(I+1)).LT.0.0.OR.GA2(I+2)/DABS(GA2(I+2)).
     *LT.0.0) THEN
      AAT(I,I)=ST(I+1)
      AAT(I,I+2+N)=ST(I+2+M)
      GO TO 440
      END IF
      AAT(I,I)=ST(I+2)
      AAT(I,I+1+N)=ST(I+1+M)
```

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        FORTRAN77 EX    V12L10    TEMPRT        DATE 92-09-21  TIME 20:42:03

00000130 440    CONTINUE
         C
00000131        DO 450 I=1,M
00000132        GX2(I)=GA2(I)*D(I)/C(3)/C(13)
00000133        AAT(I+N,I+N)=CPO(I)/C(7)*GX2(I)
00000134        AAT(I+N,NI(I))=-CPN(NI(I))/C(7)*GX2(I)
00000135        IF(GA2(5)/ABS(GA2(5)).GE.0.0)
               *AAT(5+N,NI(5))=-CPN(NI(5))/C(7)*GX2(4)
00000136        IF(GA2(5)/ABS(GA2(5)).LT.0.0)
               *AAT(5+N,NI(5))=-CPN(NI(5))/C(7)*GX2(6)
00000137        IF(GA2(11)/ABS(GA2(11)).GE.0.0)
               *AAT(11+N,NI(11))=-CPN(NI(11))/C(7)*GX2(10)
00000138        IF(GA2(11)/ABS(GA2(11)).LT.0.0)
               *AAT(11+N,NI(11))=-CPN(NI(11))/C(7)*GX2(12)
00000139        IF(GA2(I)/DABS(GA2(I)).LT.0.0) AAT(I+N,2*M)=-AT(I)
00000140        IF(GA2(I)/DABS(GA2(I)).GE.0.0) AAT(I+N,2*M)=AT(I)
00000141 450    CONTINUE
         C
         C***********    TO SOLVE MATRIX    ****************************************
         C
00000142        CALL GAUELD (AAT,2*M-1,2*M-1,2*M,1.0E-10,ILL)
00000143        IF (ILL.EQ.0) GO TO 1
00000144        WRITE(6,*) 'GAUELD AT TEMPRT ; L, ILL   ',L,ILL
00000145        STOP
00000146 1      DO 2 JJ=2*M,2*M
00000147        DO 3 I=1,N
00000148        TX1(I)=(TN1(I)+273.15)/C(2)
00000149        TN1(I)=AAT(I,JJ)*C(2) - 273.15
00000150 3      CONTINUE
00000151        DO 2 I=1,M
00000152        TX1(I+N)=(TO1(I)+273.15)/C(2)
00000153        TO1(I)=AAT(I+N,JJ)*C(2) - 273.15
00000154 2      CONTINUE
         C
00000155        EPS=1.0E-3
00000156        TTA=0.0
00000157        DO 55 I=1,2*M-1
00000158        TA(I)=0.0
00000159 55     CONTINUE
00000160        DO 50 I=1,2*M-1
00000161        TA(I)=DABS((AAT(I,2*M)-TX1(I))/TX1(I))
00000162 50     CONTINUE
00000163        DO 56 I=1,2*M-2
00000164        IF (TA(I+1).GE.TA(I)) TTA=TA(I+1)
00000165        IF (TA(I+1).LT.TA(I)) TTA=TA(I)
00000166 56     CONTINUE
00000167        IF (TTA.LE.EPS) GO TO 40
         C
00000168        DO 210 JJ=1,2*M-1
00000169        TX1(JJ)=TX1(JJ)+0.1*(AAT(JJ,2*M)-TX1(JJ))
00000170 210    CONTINUE
00000171        DO 215 I=1,N
00000172        TN1(I)=TX1(I)*C(2) - 273.15
00000173 215    CONTINUE
00000174        DO 225 I=1,M
00000175        TO1(I)=TX1(I+N)*C(2) - 273.15
00000176 225    CONTINUE
00000177        DO 240 JJ=1,M
00000178        SS=4.0*LAM(JJ)*NU(JJ)*H(JJ)/DABS(GA2(JJ))/D(JJ)**2/CP(JJ)
00000179        TA1(JJ)=TWA(JJ)+(TX1(NI(JJ))*C(2)-273.15-TWA(JJ))/SS
```

```
FORTRAN77 EX    V12L10   TEMPRT        DATE 92-09-21  TIME 20:42:03

     *              *(1.0-1.0*EXP(-SS))
 240  CONTINUE
 200  CONTINUE
C
C******************    CONVERGED !!!    *********************************
C
 40   DO 60 I=1,N
      TN2(I)=AAT(I,2*M)*C(2) - 273.15
      TN1(I)=TN2(I)
 60   CONTINUE
      DO 65 I=1,M
      TO2(I)=AAT(I+N,2*M)*C(2) - 273.15
      TO1(I)=TO2(I)
      SS=4.0*LAM(I)*NU(I)*H(I)/DABS(GA2(I))/D(I)**2/CP(I)
      TA2(I)=TWA(I)+(TN2(NI(I))-TWA(I))/SS*(1.0-1.0*EXP(-SS))
      TA1(I)=TA2(I)
 65   CONTINUE
      RETURN
      END
```

```
        FORTRAN77 EX    V12L10                 DATE 92-09-21  TIME 20:42:03
         C
         C*******************************************************************
         C*****                                                         *****
         C*****        TO SOLVE CONCENTRATION OF NODE AND BRANCH OUTLET *****
         C*****                                                         *****
00000001                       SUBROUTINE GASPEC ( KK )
         C*****                                                         *****
         C*******************************************************************
         C
00000002       IMPLICIT REAL*8 (A-H,O-Z)
00000003       PARAMETER (N=26, M=27, K=5, J=200, RG=8.314, PI=3.141592654 )
         C
00000004       DIMENSION H(M),D(M),Y(M),F(M),CAT(M),
              *TI1(M),TI2(M),TO1(M),TO2(M),TA1(M),TA2(M),TN1(N),TN2(N),TWA(M),
              *P1(N),P2(N),PN1(N),PN2(N),PA1(M),PA2(M),
              *GA1(M),GA2(M),GA(M),GGT(M),TTAT(M),PP(N),PPT(N),PAT(M),WAAT(M,K),
              *DI(M,K),CP(M),DEI(M),DEO(M),DEA1(M),DEAT(M),CPT(M),
              *WN1(N,K),WN2(N,K),CS(2*M),Q(M),AVEMOL(M),CPO(M),CPN(M),
              *RE(M),GR(M),PR(M),SC(M,K),SH(M,K),SI(M,K),WWA(M,K),
              *WI1(M,K),WI2(M,K),WO1(M,K),WO2(M,K),WA1(M,K),WA2(M,K),
              *AW(M,K),BW(M,K),CW(M,K),DW(M,K),AAW(2*M-1,2*M),SW(2*M,K),
              *C(13),BAT(M,K),XW(K),GX2(M),NI(M),NO(M),
              *WX1(2*M-1,K),WX2(2*M-1,K),TA(K)
00000005       REAL*8 NNI(M),NNO(M),MU(M),LAM(M),NU(M),MOLW(K+1)
00000006       COMMON/SIZE/H,D,Y,F,NNI,NNO,CAT,DT
              *       /TEMP/TI1,TI2,TO1,TO2,TA1,TA2,TN1,TN2,TWA,TTAT
              *       /PRES/P1,P2,PN1,PN2,PA1,PA2,PP,PPT,PAT
              *       /COMP/WI1,WI2,WO1,WO2,WA1,WA2,WN1,WN2,WAAT,WWA
              *       /FLOW/GA1,GA2,GA,GGT,
              *       /QUAL/DI,CP,CPT,CPO,CPN,MU,LAM,DEI,DEO,DEA1,DEAT
              *       /MLWG/MOLW,AVEMOL,C
              *       /REFE/RE,GR,PR,NU,SC,SH,Q
         C
00000007       DO 200 L=1,J
00000008       DO 30 JJ=1,2*M-1
00000009       DO 30 KJ=1,2*M
00000010       AAW(JJ,KJ)=0.0
00000011 30    CONTINUE
00000012       DO 150 I=1,M
00000013       IF(GA2(I)/DABS(GA2(I)).LT.0.0) THEN
00000014       NI(I)=NNO(I)
00000015       NO(I)=NNI(I)
00000016       END IF
00000017       IF (GA2(I)/DABS(GA2(I)).GE.0.0) THEN
00000018       NI(I)=NNI(I)
00000019       NO(I)=NNO(I)
00000020       END IF
00000021       DO 150 JJ=1,K
00000022       AW(I,JJ) = 0.0
00000023       BW(I,JJ) = 0.0
00000024       CW(I,JJ) = 0.0
00000025       DW(I,JJ) = 0.0
00000026       WI2(I,JJ)=0.0
00000027       WO2(I,JJ)=0.0
00000028       WN2(NI(I),JJ)=0.0
00000029       IF (GA2(1)/DABS(GA2(1)).GE.0.0) THEN
00000030       WN1(1,1)=0.0
00000031       WN1(1,2)=0.233
00000032       WN1(1,3)=0.0
00000033       WN1(1,4)=0.0
```

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           FORTRAN77 EX    V12L10    GASPEC       DATE 92-09-21  TIME 20:42:03

00000034         WN1(1,5)=0.767
00000035         END IF
00000036         IF (GA2(M)/DABS(GA2(M)).LT.0.0) THEN
00000037         WN1(N,1)=0.0
00000038         WN1(N,2)=0.233
00000039         WN1(N,3)=0.0
00000040         WN1(N,4)=0.0
00000041         WN1(N,5)=0.767
00000042         END IF
00000043         WI1(I,JJ)=WN1(NI(I),JJ)
00000044 150     CONTINUE
         C
         C****** MASS TRANSFER COEFFICIENT AND GENERATION/DISAPPEARANCE TERM ****
         C
00000045         DO 350 I=1,M
00000046         AKPLS = 7.0E+9*EXP(-199720.0/RG/(TA2(I)+273.15))
00000047         RPLS  = AKPLS*DEA1(I)*(DEA1(I)/MOLW(2))**0.5*WA1(I,3)
                1         *WA1(I,2)**0.5
00000048         SI(I,1) = 0.0
00000049         SI(I,2) = -0.5*RPLS
00000050         SI(I,3) = -RPLS
00000051         SI(I,4) = RPLS
00000052         SI(I,5) = 0.0
00000053         Q(I)=D(I)**2/(C(2)*C(13)*C(3)*C(7))*5.660E5*RPLS/MOLW(4)
00000054         DO 350 JJ=1,K
00000055         SC(I,JJ)=MU(I)/DI(I,JJ)/DEA1(I)
00000056         SH(I,JJ) = AMTC ( RE(I), SC(I,JJ), H(I)/D(I) )
00000057         BAT(I,JJ) = SH(I,JJ)*DI(I,JJ)/D(I)
00000058         BW(I,JJ) = 0.0
00000059         CW(I,JJ) = 0.0
00000060           IF ( I.EQ.5.OR.I.EQ.11 )  THEN
00000061         BW(I,JJ)=4.0*SH(I,JJ)*DI(I,JJ)*H(I)/D(I)/C(13)
00000062         IF(KK.EQ.1) CW(I,JJ)=BW(I,JJ)
00000063           ENDIF
00000064         IF(KK.EQ.2) CW(I,JJ)=BW(I,JJ)+H(I)*D(I)/DT/C(13)
00000065         DW(I,JJ)=SI(I,JJ)*D(I)*H(I)/C(3)/C(13)
00000066         IF(KK.EQ.2) DW(I,JJ)=DW(I,JJ)+H(I)*D(I)/DT/C(13)*DEAT(I)/C(3)
                **WAAT(I,JJ)
00000067         AW(I,JJ)=AW(I,JJ)+BW(I,JJ)*WWA(I,JJ)*DEA1(I)/C(3)
00000068         AW(I,JJ)=AW(I,JJ)-CW(I,JJ)*WA1(I,JJ)*DEA1(I)/C(3)
00000069         AW(I,JJ)=AW(I,JJ)+DW(I,JJ)
00000070 350     CONTINUE
         C
         C**************** COEFFICIENTS OF MATRIX ****************************
         C
00000071         DO 110 I=1,M
00000072         DO 110 JJ=1,K
00000073         SW(I,JJ)=PI/4.0*D(I)**2*DABS(GA2(I))
00000074         IF(GA2(5)/DABS(GA2(5)).GE.0.0)
                *SW(5,JJ)=PI/4.0*D(5)**2*DABS(GA2(4))
00000075         IF(GA2(5)/DABS(GA2(5)).LT.0.0)
                *SW(5,JJ)=PI/4.0*D(5)**2*DABS(GA2(6))
00000076         IF(GA2(11)/DABS(GA2(11)).GE.0.0)
                *SW(11,JJ)=PI/4.0*D(11)**2*DABS(GA2(10))
00000077         IF(GA2(11)/DABS(GA2(11)).LT.0.0)
                *SW(11,JJ)=PI/4.0*D(11)**2*DABS(GA2(12))
00000078 110     CONTINUE
00000079         DO 120 I=M+1,2*M
00000080         DO 120 JJ=1,K
00000081         SW(I,JJ)=-PI/4.0*D(I-M)**2*DABS(GA2(I-M))
```

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```
 120  CONTINUE
      DO 500 JJ=2,4
      DO 550 II=1,2*M-1
      DO 550 IJ=1,2*M
      AAW(II,IJ)=0.0
 550  CONTINUE
      IF(GA2(1)/DABS(GA2(1)).GE.0.0)THEN
      IF(JJ.EQ.1) AAW(1,2*M)=0.0
      IF(JJ.EQ.2) AAW(1,2*M)=0.233
      IF(JJ.EQ.3) AAW(1,2*M)=0.0
      IF(JJ.EQ.4) AAW(1,2*M)=0.0
      IF(JJ.EQ.5) AAW(1,2*M)=0.767
      AAW(1,1)=1.0
      END IF
      IF(GA2(1)/DABS(GA2(1)).LT.0.0) THEN
      AAW(1,1)=1.0
      AAW(1,M)=-1.0
      END IF
      IF(GA2(M)/DABS(GA2(M)).LT.0.0) THEN
      IF(JJ.EQ.1) AAW(N,2*M)=0.0
      IF(JJ.EQ.2) AAW(N,2*M)=0.233
      IF(JJ.EQ.3) AAW(N,2*M)=0.0
      IF(JJ.EQ.4) AAW(N,2*M)=0.0
      IF(JJ.EQ.5) AAW(N,2*M)=0.767
      AAW(N,N)=1.0
      END IF
      IF(GA2(M)/DABS(GA2(M)).GE..0) THEN
      AAW(N,N)=1.0
      AAW(N,N+M)=-1.0
      END IF
      DO 395 I=1,2*M
      CS(I)=1.0
 395  CONTINUE
      DO 405 I=2,14,6
      IF(GA2(I)/DABS(GA2(I)).GE.0.0) CS(I+M)=0.0
      IF(GA2(I)/DABS(GA2(I)).LT.0.0) CS(I)=0.0
      IF(GA2(1)/DABS(GA2(1)).GE.0.0) CS(1)=0.0
      IF(GA2(1)/DABS(GA2(1)).LT.0.0) CS(M+1)=0.0
      AAW(2,2)=CS(1)*SW(1,JJ)+CS(2)*SW(2,JJ)+CS(8)*SW(8,JJ)
     *+CS(14)*SW(14,JJ)
      AAW(2,I+N)=CS(I+M)*SW(I+M,JJ)
      AAW(2,M)=CS(M+1)*SW(M+1,JJ)
 405  CONTINUE
      DO 415 I=3,7
      IF(GA2(I)/DABS(GA2(I)).LT.0.0.OR.GA2(I-1)/DABS(GA2(I-1)).LT.0.0
     *) THEN
      AAW(I,I)=SW(I-1,JJ)
      AAW(I,I+N)=SW(I+M,JJ)
      GO TO 415
      END IF
      AAW(I,I)=SW(I,JJ)
      AAW(I,I+N-1)=SW(I+M-1,JJ)
 415  CONTINUE
      DO 425 I=8,12
      IF(GA2(I)/DABS(GA2(I)).LT.0.0.OR.GA2(I+1)/DABS(GA2(I+1)).
     *LT.0.0) THEN
      AAW(I,I)=SW(I,JJ)
      AAW(I,I+1+N)=SW(I+1+M,JJ)
      GO TO 425
      END IF
```

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          AAW(I,I)=SW(I+1,JJ)
          AAW(I,I+N)=SW(I+M,JJ)
    425   CONTINUE
          DO 435 I=13,17
          IF(GA2(I+1)/DABS(GA2(I+1)).LT.0.0.OR.GA2(I+2)/DABS(GA2(I+2)).
         *LT.0.0) THEN
          AAW(I,I)=SW(I+1,JJ)
          AAW(I,I+2+N)=SW(I+2+M,JJ)
          GO TO 435
          END IF
          AAW(I,I)=SW(I+2,JJ)
          AAW(I,I+1+N)=SW(I+1+M,JJ)
    435   CONTINUE
C
          IF(GA2(7)/DABS(GA2(7)).GE.0.0) CS(7)=0.0
          IF(GA2(7)/DABS(GA2(7)).LT.0.0) CS(7+M)=0.0
          IF(GA2(13)/DABS(GA2(13)).GE.0.0) CS(13)=0.0
          IF(GA2(13)/DABS(GA2(13)).LT.0.0) CS(13+M)=0.0
          IF(GA2(19)/DABS(GA2(19)).GE.0.0) CS(19)=0.0
          IF(GA2(19)/DABS(GA2(19)).LT.0.0) CS(19+M)=0.0
          IF(GA2(20)/DABS(GA2(20)).GE.0.0) CS(20+M)=0.0
          IF(GA2(20)/DABS(GA2(20)).LT.0.0) CS(20)=0.0
          AAW(18,18)=CS(7)*SW(7,JJ)+CS(13)*SW(13,JJ)+CS(19)*SW(19,JJ)
         *+CS(20)*SW(20,JJ)
          AAW(18,7+N)=CS(7+M)*SW(7+M,JJ)
          AAW(18,13+N)=CS(13+M)*SW(13+M,JJ)
          AAW(18,19+N)=CS(19+M)*SW(19+M,JJ)
          AAW(18,20+N)=CS(20+M)*SW(20+M,JJ)
C
          DO 445 I=19,25
          IF(GA2(I+1)/DABS(GA2(I+1)).LT.0.0.OR.GA2(I+2)/DABS(GA2(I+2)).
         *LT.0.0) THEN
          AAW(I,I)=SW(I+1,JJ)
          AAW(I,I+2+N)=SW(I+2+M,JJ)
          GO TO 445
          END IF
          AAW(I,I)=SW(I+2,JJ)
          AAW(I,I+1+N)=SW(I+1+M,JJ)
    445   CONTINUE
          DO 455 I=1,M
          GX2(I)=GA2(I)*D(I)/C(3)/C(13)
          AAW(I+N,I+N)=GX2(I)
          AAW(I+N,NI(I))=-GX2(I)
          IF(GA2(5)/ABS(GA2(5)).GE.0.0)
         *AAW(5+N,NI(5))=-GX2(4)
          IF(GA2(5)/ABS(GA2(5)).LT.0.0)
         *AAW(5+N,NI(5))=-GX2(6)
          IF(GA2(11)/ABS(GA2(11)).GE.0.0)
         *AAW(11+N,NI(11))=-GX2(10)
          IF(GA2(11)/ABS(GA2(11)).LT.0.0)
         *AAW(11+N,NI(11))=-GX2(12)
          IF(GA2(I)/DABS(GA2(I)).LT.0.0) AAW(I+N,2*M)=-AW(I,JJ)
          IF(GA2(I)/DABS(GA2(I)).GE.0.0) AAW(I+N,2*M)=AW(I,JJ)
    455   CONTINUE
C
          DO 90 I=1,M-1
          IF(DABS(WA1(I,JJ)).GT.DABS(WA1(I+1,JJ)))
         *XW(JJ)=DABS(WA1(I,JJ))
    90    CONTINUE
          IF(XW(JJ).EQ.0.0) GO TO 500
```

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C
C************   TO SOLVE MATRIX   ***************************************
C
      CALL GAUELD (AAW,2*M-1,2*M-1,2*M,1.0E-10,ILL)
      IF (ILL.EQ.0) GO TO 1
      WRITE(6,*) 'GAUELD AT GASPEC ; L, ILL  ',L,ILL
      STOP
1     DO 2 JK=2*M,2*M
      DO 3 I=1,N
      WX1(I,JJ)=WN1(I,JJ)
      WX2(I,JJ)=AAW(I,JK)
      WN1(I,JJ)=AAW(I,JK)
      AAW(I,JK)=0.0
3     CONTINUE
      DO 2 I=N+1,N+M
      WX1(I,JJ)=WO1(I-N,JJ)
      WX2(I,JJ)=AAW(I,JK)
      WO1(I-N,JJ)=AAW(I,JK)
      AAW(I,JK)=0.0
    2 CONTINUE
C
      EPS=1.0E-5
      DO 50 I=1,2*M-2
      IF (DABS(WX2(I+1,JJ)-WX1(I+1,JJ)).GT.
     *DABS(WX2(I,JJ)-WX1(I,JJ)))  THEN
      TA(JJ)=DABS(WX2(I+1,JJ)-WX1(I+1,JJ))
      ENDIF
50    CONTINUE
500   CONTINUE
      DO 70 JJ=1,K-1
      IF(TA(JJ+1).GT.TA(JJ)) TTA=TA(JJ+1)
70    CONTINUE
      IF (TTA.LE.EPS) GO TO 40
C
      DO 215 I=1,2*M-1
      DO 215 JJ=1,K
      IF(WX2(I,JJ).LT.0.0) WX2(I,JJ)=0.0
215   CONTINUE
      DO 210 I=1,2*M-1
      WX2(I,1)=0.0
      WX2(I,5)=1.0-WX2(I,2)-WX2(I,3)-WX2(I,4)
      DO 210 JJ=1,K
      WX1(I,JJ)=WX1(I,JJ)+0.3*(WX2(I,JJ)-WX1(I,JJ))
      IF(GA2(1)/DABS(GA2(1)).GE.0.0) THEN
      WX1(1,1)=0.0
      WX1(1,2)=0.233
      WX1(1,3)=0.0
      WX1(1,4)=0.0
      WX1(1,5)=0.767
      END IF
      IF(GA2(M)/DABS(GA2(M)).LT.0.0) THEN
      WX1(N,1)=0.0
      WX1(N,2)=0.233
      WX1(N,3)=0.0
      WX1(N,4)=0.0
      WX1(N,5)=0.767
      END IF
210   CONTINUE
      DO 230 I=1,N
      DO 230 JJ=1,K
```

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          WN1(I,JJ)=WX1(I,JJ)
          WN1(I,1)=0.0
          WN1(I,5)=1.0-WX1(I,2)-WX1(I,3)-WX1(I,4)
  230     CONTINUE
          DO 245 I=N+1,N+M
          DO 245 JJ=1,K
          WO1(I-N,JJ)=WX1(I,JJ)
          WO1(I-N,1)=0.0
          WO1(I-N,5)=1.0-WO1(I-N,2)-WO1(I-N,3)-WO1(I-N,4)
  245     CONTINUE
          DO 255 I=1,M
          DO 255 JJ=1,K
          SS=4.0*BAT(I,JJ)*H(I)*DEA1(I)/ABS(GA2(I))/D(I)
          WA1(I,JJ)=WWA(I,JJ)+(WN1(NI(I),JJ)-WWA(I,JJ))/SS*
         *(1.0-1.0*EXP(-SS))
  255     CONTINUE
  200     CONTINUE
            WRITE(6,*) '*****  ITERATION TIME IS OVER'
         1             ,' AT GASPEC SUBROUTINE !!  ;  ERR = ',TTA,'  *****'
C
C***************     CONVERGED !!!    ***********************************
C
  40      DO 60 I=1,2*M-1
          DO 60 JJ=1,K
          IF(WX2(I,JJ).LT.0.0) WX2(I,JJ)=0.0
  60      CONTINUE
          DO 65 I=1,2*M-1
          WX2(I,1)=0.0
          WX2(I,5)=1.0-WX2(I,1)-WX2(I,2)-WX2(I,3)-WX2(I,4)
          IF (GA2(1)/DABS(GA2(1)).GE.0.0) THEN
          WX2(1,1)=0.0
          WX2(1,2)=0.233
          WX2(1,3)=0.0
          WX2(1,4)=0.0
          WX2(1,5)=0.767
          END IF
          IF (GA2(M)/DABS(GA2(M)).LT.0.0) THEN
          WX2(N,1)=0.0
          WX2(N,2)=0.233
          WX2(N,3)=0.0
          WX2(N,4)=0.0
          WX2(N,5)=0.767
          END IF
  65      CONTINUE
          DO 75 I=1,N
          DO 75 JJ=1,K
          WN2(I,JJ)=WX2(I,JJ)
  75      WN1(I,JJ)=WN2(I,JJ)
          DO 95 I=1,M
          DO 95 JJ=1,K
          WO2(I,JJ)=WX2(I+N,JJ)
          WO1(I,JJ)=WO2(I,JJ)
          SS=4.0*BAT(I,JJ)*H(I)*DEA1(I)/DABS(GA2(I))/D(I)
          WA2(I,JJ)=WWA(I,JJ)+(WN2(NI(I),JJ)-WWA(I,JJ))/SS*
         *(1.0-1.0*EXP(-SS))
  95      WA1(I,JJ)=WA2(I,JJ)
C
          RETURN
          END
```

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         C
         C***********************************************************************
         C*****                                                            *****
         C*****     SUBROUTINE PROGRAM FOR MASS FRACTION ON GRAPHITE WALL   *****
         C*****                                                            *****
00000001            SUBROUTINE BNDCHM  ( RE, SC, XBYD, D, RHOO, AMUO, RHO,
              1                          OMGB, TW, P, AM, OMGW, GM1 )
         C*****                                                            *****
         C***********************************************************************
         C
00000002       IMPLICIT REAL*8 (A-H,O-Z)
00000003       PARAMETER ( RG=8.314, K=5, EPS=1.0E-6, XIO=1.0E-2, XIMIN=1.0E-8 )
00000004       DIMENSION SH(3), SC(K), OMGB(K), OMGW(K), AMOL(K+1)
00000005       COMMON /MLWG/AMOL
         C
00000006       SH(1) = AMTC ( RE, SC(2), XBYD )
00000007       SH(2) = AMTC ( RE, SC(3), XBYD )
00000008       SH(3) = AMTC ( RE, SC(4), XBYD )
00000009       TWK   = TW + 273.15
00000010       F     = 800.0*EXP(-6200.0/TWK)
00000011       AN    = 0.75
         C
00000012       C1    = -2560.0*EXP(-142000.0/RG/TWK)*(P/1.013E5)**0.5
              1          *(AM/0.2095/AMOL(2))**AN
00000013       C2    = -44.5*EXP(-162710.0/RG/TWK)
00000014       AO2L  =-SH(1)*RHO/SC(2)
00000015       ACOL  =-SH(2)*RHO/SC(3)
00000016       ACO2L =-SH(3)*RHO/SC(4)
00000017       AO2R  = AMOL(2)/AMOL(6)*D*D/RHOO/AMUO*(2.0+F)/(2.0+2.0*F)*C1
00000018       ACOR1 =-AMOL(3)/AMOL(6)*D*D/RHOO/AMUO*F/(1.0+F)*C1
00000019       ACOR2 =-2.0*AMOL(3)/AMOL(6)*C2*D*D/RHOO/AMUO
00000020       ACO2R1=-AMOL(4)/AMOL(6)/RHOO/AMUO*D*D/(1.0+F)*C1
00000021       ACO2R2= AMOL(4)/AMOL(6)*C2*D*D/RHOO/AMUO
         C
00000022       XI       = XIO
00000023         DO 100 I=1,20
00000024       FNC      = AO2R*XI**AN + AO2L*XI - AO2L*OMGB(2)
00000025       FNCD     = AO2R*AN*XI**(AN-1.0) + AO2L
00000026       XIP1     = XI - FNC/FNCD
00000027       ERR      = ABS( (XIP1-XI)/XI )
00000028         IF ( ERR.LT.EPS )              GO TO 200
00000029         IF ( XIP1.LT.0.0 )  XIP1 = XIMIN
00000030       XI       = XIP1
00000031   100   CONTINUE
         C
00000032   200 OMGW(2)  = XIP1
00000033       OMGW(4)  = (-ACO2R1*OMGW(2)**AN + ACO2L*OMGB(4))/(ACO2R2+ACO2L)
00000034       OMGW(3)  = (ACOL*OMGB(3)-ACOR1*OMGW(2)**AN-ACOR2*OMGW(4))/ACOL
00000035       OMGW(1)  = OMGB(1)
00000036       OMGW(5)  = OMGB(5)
00000037       GM1      = -C1*OMGW(2)**AN - C2*OMGW(4)
         C
00000038       RETURN
00000039       END
```

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        C
        C**********************************************************************
        C*****                                                           *****
        C*****     FUNCTION PROGRAM FOR CALCULATION OF FRICTION FACTOR   *****
        C*****                                                           *****
00000001                  FUNCTION  FRIC  ( RE, XBYD )
        C*****                                                           *****
        C**********************************************************************
        C
00000002      IMPLICIT REAL*8 (A-H,O-Z)
        C
00000003      FAPP(X,Y)=( 3.44/X**0.5 + (1.25/4.0/X+16.0-3.44/X**0.5)
             1          /(1.0+2.1E-4/X/X) ) / Y
        C
00000004      X1   = 0.000001
00000005      X2   = XBYD
00000006      FRIC = ( X2*FAPP(X2,RE) - X1*FAPP(X1,RE) )/( X2-X1 )
        C
00000007      RETURN
00000008      END
```

```
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         C
         C*************************************************************************
         C*****                                                               *****
         C*****    FUNCTION PROGRAM FOR CALCULATION OF HEAT TRANSFER.         *****
         C*****                                                               *****
00000001                   FUNCTION  HTC ( RE, PR, XBYD )
         C*****                                                               *****
         C*************************************************************************
         C
00000002       IMPLICIT REAL*8 (A-H,O-Z)
         C
00000003       ANU1 (X) = 1.615*X**(-0.333333) - 0.7
00000004       ANU2 (X) = 1.615*X**(-0.333333) - 0.2
00000005       ANU3 (X) = 3.657 + 0.0499/X
         C
00000006       X1     = 0.00001
00000007       X2     = XBYD
00000008         IF ( RE.LE.1.0.OR.PR.LE.1.0E-4 ) THEN
00000009       HTC    = 1.0
00000010       RETURN
00000011         ENDIF
00000012       XAST1 = X1/RE/PR
00000013       XAST2 = X2/RE/PR
00000014         IF ( XAST1.LE.0.005 )                        ANUX1=ANU1(XAST1)
00000015         IF ( XAST1.GT.0.005.AND.XAST1.LT.0.03 )  ANUX1=ANU2(XAST1)
00000016         IF ( XAST1.GE.0.03  )                        ANUX1=ANU3(XAST1)
00000017         IF ( XAST2.LE.0.005 )                        ANUX2=ANU1(XAST2)
00000018         IF ( XAST2.GT.0.005.AND.XAST2.LT.0.03 )  ANUX2=ANU2(XAST2)
00000019         IF ( XAST2.GE.0.03  )                        ANUX2=ANU3(XAST2)
         C
00000020       CND1 = 1.0
00000021       CND2 = 1.0
00000022       CND  = 1.0
00000023       DT1  = 1.0
00000024       DT2  = 1.0
00000025       DT   = 1.0
00000026       HTC = ( X2*ANUX2*DT2*CND2 - X1*ANUX1*DT1*CND1 )/( X2 - X1 )
              1          /DT/CND
         C
00000027       RETURN
00000028       END
```

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         C
         C**********************************************************************
         C*****                                                            *****
         C*****    FUNCTION PROGRAM FOR CALCULATION OF MASS TRANSFER       *****
         C*****                                                            *****
00000001                     FUNCTION  AMTC ( RE, SC, XBYD )
         C*****                                                            *****
         C**********************************************************************
         C
00000002       IMPLICIT REAL*8 (A-H,O-Z)
         C
00000003       SH1 (X) = 1.615*X**(-0.333333) - 0.7
00000004       SH2 (X) = 1.615*X**(-0.333333) - 0.2
00000005       SH3 (X) = 3.657 + 0.0499/X
         C
00000006       X1    = 0.00001
00000007       X2    = XBYD
00000008         IF ( RE.LE.1.0.OR.SC.LE.1.0E-4 ) THEN
00000009       AMTC  = 1.0
00000010       RETURN
00000011         ENDIF
00000012       XAST1 = X1/RE/SC
00000013       XAST2 = X2/RE/SC
00000014         IF ( XAST1.LE.0.005 )                     SHX1=SH1(XAST1)
00000015         IF ( XAST1.GT.0.005.AND.XAST1.LT.0.03 ) SHX1=SH2(XAST1)
00000016         IF ( XAST1.GE.0.03  )                     SHX1=SH3(XAST1)
00000017         IF ( XAST2.LE.0.005 )                     SHX2=SH1(XAST2)
00000018         IF ( XAST2.GT.0.005.AND.XAST2.LT.0.03 ) SHX2=SH2(XAST2)
00000019         IF ( XAST2.GE.0.03  )                     SHX2=SH3(XAST2)
         C
00000020       DIF1 = 1.0
00000021       DIF2 = 1.0
00000022       DIF  = 1.0
00000023       DW1  = 1.0
00000024       DW2  = 1.0
00000025       DW   = 1.0
00000026       AMTC = ( X2*SHX2*DW2*DIF2 - X1*SHX1*DW1*DIF1 )/( X2 - X1 )
              1         /DW/DIF
         C
00000027       RETURN
00000028       END
END OF COMPILATION,HIGHEST SEVERITY CODE=00
```