PADLOC, A ONE-DIMENSIONAL COMPUTER PROGRAM FOR CALCULATING COOLANT AND PLATEOUT FISSION PRODUCT CONCENTRATIONS

by

W. W. HUDRITSCH and P. D. SMITH

Prepared under
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This report was prepared as a part of the ERDA-funded HTGR Safety Research Task. It fulfills a major task milestone of documenting a newly developed PCRV plateout code developed for the analysis of core heatup accidents. The scope of the report is restricted to the assumptions, equations, and solution techniques of the first operational version of the computer program. The data base, application of the code to core heatup accidents, and comparisons with previous methods will be addressed in a separate report as a future milestone.
ABSTRACT

The one-dimensional computer program PADLOC is designed to analyze steady-state and time-dependent plateout of fission products in an arbitrary network of pipes. The problem solved is one of mass transport of impurities in a fluid, including the effects of sources in the fluid and in the plateout surfaces, convection along the flow paths, decay, adsorption on surfaces (plateout), and desorption from surfaces. These phenomena are governed by a system of coupled, nonlinear partial differential equations. The solution is achieved by a) linearizing the equations about an approximate solution, employing a Newton Raphson iteration technique, b) employing a finite difference solution method with an implicit time integration, and c) employing a substructuring technique to logically organize the systems of equations for an arbitrary flow network.
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1. DESCRIPTION OF PROBLEM

The safety of high-temperature gas-cooled reactors (HTGRs), measured in terms of the radiological consequences of fission product release during postulated accidents, is being continually evaluated for both licensing efforts and probabilistic risk assessments. Information required to describe and analyze an accident includes the logical order of discrete event sequences and the mathematical models of the plant transient behavior. Using the methodology of event tree diagramming and probabilistic analysis, the ERDA-funded Accident Initiation and Progression Analysis (AIPA) Task (PA-51 189a No. 00574) has been instrumental in identifying areas and priorities of safety research which can most significantly affect or verify the safety assessment.

The AIPA work to date, described in Ref. 1, determined that an unrestricted core heatup is the highest risk* accident for an HTGR. Associated with this postulated event, the phenomena of time-dependent fission product release from the core and plateout (adsorption) on internal PCRV surfaces were ranked as high priority research tasks by virtue of their prominent contribution to consequence uncertainties. Also, the PCRV plateout assumptions were the subject of extensive AIPA reviewer comments as discussed in Volume VIII of Ref. 1. Thus, the need for improved accuracy in predicting plateout is of crucial importance for AIPA risk assessments.

PCRV plateout predictions in Ref. 1 were based on empirical constants from sparse experimental data. No computer model was available for application to these extreme accident conditions, although computer codes such as PAD at GAC and others in France and Germany exist for predicting plateout under operating conditions. In FY-76, effort was initiated under the HTGR Safety Research Task (PA-51 189a No.00577) to develop a computer program to calculate the time-dependent spatial

*Risk is defined here as the product of the consequence of an event and the probability of its occurrence per reactor year.
distribution of fission products during a core heatup event. In addition, to maintain commonality and consistency with steady-state plateout analyses, it was desired to develop the code so that it would be applicable to steady-state operating conditions. This was achieved by basing the new code on the same differential equations solved by the existing PAD code\(^2\) and developing a new code with a much more versatile and efficient solution method. This report presents a technical description of the first operating version of this new code, including a user's manual. Application of the code to specific cases is outside the present scope.

The fission product contamination in the coolant and on the surfaces of the coolant circuit and the PCRV depends mainly on the release from the core, the flow of the coolant, and the mass transfer characteristics between the coolant and the conduit surfaces. In addition, contamination levels depend on precursors and decay. More technically, the problem to be solved is one of mass transport of impurities in a fluid, including the effects of

- sources in the coolant,
- sources on the surfaces,
- convection along the flow path,
- decay,
- plateout (adsorption on surfaces), and
- desorption from surfaces.

The problem is assumed to be one-dimensional, i.e., parameters are allowed to vary only along the direction of the fluid flow. For general application to a variety of operating and accident conditions, a model with the following characteristics is required:

- The geometry is idealized as an arbitrary network of pipes.
- Boundary conditions and mixing conditions, which may be time-dependent, control the behavior at pipe junctions.
- Time-dependent flow and mass transfer parameters are computed from input data such as coolant mass flow, temperature, pressure, hydraulic diameter, wall temperature, etc.
- The unknowns to be found are the space and time variations of the impurity concentrations in the coolant and on the plateout surfaces.
Until recently, this type of problem has been solved at GAC with the PAD code. This code has two disadvantages that restrict its usefulness. First, PAD employs an explicit time integration method. This necessitates very short time steps in order to avoid numerical instability. A PAD analysis of any reasonable irradiation history would require unacceptable computer running times. Second, PAD is restricted to the analysis of a single closed loop. The modeling of certain accident conditions, e.g., a postulated loss of forced cooling (LOFC) accident, requires the consideration of more complicated networks. The newly developed PADLOC (Plateout Activity Distribution for Loss of Circulation) code employs an implicit solution method and considers an arbitrary network geometry, thereby removing both of these disadvantages.

The problem solved by PADLOC will now be described in more detail in the context of particular HTGR applications. These include both normal operating conditions and the core heatup accident. The code itself is quite general and many other applications are possible.

Figure 1 on the following page shows a schematic diagram of one steam generator loop of the primary circuit of an HTGR. During normal operation, small amounts of fission products enter the loop from the core. Part of the coolant is routed through the purification system which removes all fission products in this parallel train. In Figure 2 the coolant paths for a core heatup accident are depicted. In this case the helium circulators are out of operation, but the coolant, while being heated up by the core, may still circulate around the regular loop by natural convection. As the coolant is heated the pressure in the reactor rises until, at a specified pressure, the relief valve in the upper plenum opens and contaminated coolant escapes into the containment building. In order to estimate activity levels at any given time, the distribution of fission products along the flow paths has to be known.

From these examples it is obvious that flow paths can be complicated and interconnected. Also, coolant conditions change along the conduits and, in general, there may be sources of fission products at various places in the network.
CLEAN COOLANT

FISSION PRODUCT TRAPS OF THE HELIUM PURIFICATION SYSTEM

COOLANT AND FISSION PRODUCTS

PLENUM

FISSION PRODUCTS ENTERING THE COOLANT

CORE

PLENUM

COOLANT DIRECTION

CIRCULATOR

STEAM GENERATOR

FISSION PRODUCTS PLATING OUT

Fig. 1. Primary circuit with normal operating conditions
Fig. 2. Coolant flow for postulated loss of forced cooling accident
Section 2 of this report contains a brief description of the method employed to solve for the fission product concentrations in the coolant and on the plateout surfaces. Sections 3 through 5 give the more detailed theory of the PADLOC model. Sections 6 and 7 contain a user's manual for the PADLOC code and the results of some sample problems. Appendix A is a detailed description of the formulae used for calculating mass transfer coefficients.
2. SUMMARY OF METHOD

For reasons discussed in Ref. 3, the coolant flow paths are divided into sections or branches along which parameters such as velocity, conduit cross section, temperatures, etc., are assumed to vary smoothly. The individual branches are then connected to a global branch network resembling the actual geometry. Such networks for the conditions of Figures 1 and 2 might look like those of Figures 3 and 4.*

The method used to solve for the coolant and plateout concentrations is summarized as follows:

1. Establish the equations governing the coolant concentration for each of the branches under the assumption of known boundary conditions at the upstream ends of the branches.

2. For each branch in turn, reduce the branch equations to one linearized equation relating the concentrations at the two branch ends.

3. Transform the unknowns in the reduced equations from concentrations to impurity atom flow rates.

* It is noted that in Figure 3 there is no branch connecting the downstream end of the purification system with the upper plenum. This branch is superfluous since it would not contain any fission products.
Fig. 3. Branch network equivalent to Fig. 1
Fig. 4. Branch network equivalent to Fig. 2 (LOFC)
4. Use the transformed equations relating branch end flow rates together with
   • global boundary conditions at free upstream branch ends, and
   • mixing equations at branch connections to
     form a global system of equations.

5. Solve the global system for the branch end flow rates.

6. Transform flow rates back to coolant concentrations.

7. For each branch in turn, use the end node concentrations to solve for the interior coolant concentrations. Use the coolant concentrations to compute plateout concentration.

   In the following section we will concern ourselves with item 1, namely the equations for a single branch.
3. MASS BALANCE EQUATIONS IN A SINGLE BRANCH

3.1 PHYSICAL MODEL

A branch is defined as a length of conduit along which coolant velocity, pressure, temperatures, geometrical parameters and fission product concentrations are required to vary smoothly. Figure 5 shows a typical branch.

As an example of the physical behavior of this system, assume for the moment that the incoming coolant has zero fission product concentration, C, and that the initial surface concentration, S, is greater than zero. As the coolant moves through the pipe its fission product concentration can be expected to increase due to desorption from the plateout surface. At the same time, the surface concentration will decrease. On the other hand, if the surface concentration S is initially zero and the coolant entering from the left has a certain concentration, this concentration will decrease along the pipe due to deposition (adsorption) on the plateout surface. The surface concentration will simultaneously increase.

Due to turbulence, the coolant can be assumed to be well mixed across the channel, allowing its fission product content to be described by the bulk concentration C(x,t), atoms/cm\(^3\). An appreciable concentration gradient appears only in the thin boundary layer. The concentration jump across the boundary layer is fully described by the addition of a second variable B(x,t), atoms/cm\(^3\), which is the bulk concentration of fission products just adjacent to the plateout surface. The net diffusion flux through the boundary layer creates the surface or plateout concentration S(x,t), atoms/cm\(^2\). The relationship between B and S is governed by a sorption mechanism. Assuming a state of equilibrium, this relationship can generally be expressed as B = f(S).
C \( (x,t) \) = COOLANT BULK CONCENTRATION, ATOMS/CM\(^3\)

B \( (x,t) \) = COOLANT CONCENTRATION AT THE FILM SURFACE, ATOMS/CM\(^3\)

S \( (x,t) \) = PLATEOUT FILM CONCENTRATION, ATOMS/CM\(^2\)

v \( (x,t) \) = AVERAGE COOLANT VELOCITY, CM/SEC

A \( (x) \) = CROSS SECTION AREA, CM\(^2\)

P \( (x) \) = WETTED PERIMETER, CM

Fig. 5. Typical branch section
3.2 DIFFERENTIAL EQUATIONS FOR THE PLATEOUT AND COOLANT CONCENTRATIONS

For the purpose of establishing the differential equations for the coolant and plateout concentrations the following restrictions and assumptions are made:

1. Restriction to a single decaying fission product. Multiple species effects are beyond the scope of the present development, although it would be a straightforward extension to include them.

2. Diffusion within the plateout surface and from the surface into the pipe material is negligible.

3. Because of relatively high fluid velocities, the axial diffusion of fission products will be ignored.

4. Fission product concentrations are so low as not to affect the coolant and pipe properties.*

With these assumptions, both coolant and plateout concentrations will depend only on the time $t$, sec, and the axial distance $x$, cm, from the pipe inlet.

3.2.1 Plateout Concentration $S$

The rate of change of the surface concentration $[\partial S/\partial t$, atoms/(cm$^2$ sec)] is the difference between the total source rate and the total removal rate. Various contributions to the source and removal are discussed below.

The diffusive mass flux across the boundary layer can go in either direction and act as either a source or removal. We will adopt the convention that this diffusive flux is positive if directed from the surface into the coolant and consider it then a removal term for the plateout surface. The only source rate for the plateout surface is then a source from within the conduit wall. For an HTGR this is usually the flux of fission products from the fuel through the graphite to the coolant hole

* This may not be the case for high plateout concentrations (LOFC) where the decay heat may affect the pipe temperature.
surfaces of the core. If there is any decay and/or neutron activation from parents, this additional source may be added to the direct source. The total surface source rate, labelled \( q_s(x,t) \) [atoms/(cm\(^2\).sec)], is assumed to be given as an input parameter by the user.

Fission products are removed from the plateout surface by decay and by diffusion through the boundary layer into the bulk coolant. The diffusion flux is proportional to the difference between the boundary layer concentration \( B(x,t) \) and the bulk coolant concentration \( C(x,t) \), namely

\[
\text{flux} = h(x,t) \frac{B(x,t) - C(x,t)}{\text{cm} \cdot \text{sec}}, \quad (1)
\]

where \( h, \text{ cm/sec} \), is the gas-phase mass-transfer coefficient.

The value of \( h \) is predicted by empirical equations (similar to those used for heat transfer) and depends on the diffusion coefficient, hydraulic diameter and dimensionless parameters such as Reynolds number, Schmidt number, Grashof number, etc. Formulae for calculating \( h \) for various geometries and flow regimes are given in Appendix A.

With this information the differential equation for the surface concentration is

\[
\frac{3S(x,t)}{\partial t} = \dot{q}_s(x,t) - h(x,t)[B(x,t) - C(x,t)] - \Lambda_s S(x,t), \quad (2)
\]

where \( \Lambda_s \text{ (sec}^{-1} \) is the decay constant. Note that a capital \( \Lambda \) is used rather than the conventional \( \lambda \) to be consistent with the coolant equation to be derived later.
3.2.2 **Coolant Concentration C**

To establish the rate equation for the coolant concentration we again need the difference between total source rate and total removal rate.

3.2.2.1 **Sources**

There are several possible sources:

- a direct source, which may be realized by injecting fission products into the coolant,* and a source from the decay and activation of parent nuclides. The sum of these sources, denoted by $q_c$ [atoms/(cm$^3$·sec)], will be specified as an input parameter by the user,

- a source due to desorption of fission products from the plateout surface and transport through the boundary layer. This is the surface removal rate (Eq. (1)) converted to a source rate per unit volume:

  \[
  \text{source rate} = \frac{P(x)}{A(x)} h(x,t) \left[ B(x,t) - C(x,t) \right].
  \]

3.2.2.2 **Removal Rates**

Fission products as before, are removed by decay with the decay constant $\lambda_s$. In the coolant one must also consider axial convection. The convection term is determined as follows: The number of fission product atoms entering the volume element $A(x)dx$ at position $x$ per unit time is

\[
\phi(x) = v(x,t) A(x) C(x,t),
\]

and at position $x + dx$ the number leaving the element is

\[
\phi(x + dx).
\]

* Useful for certain plateout experiments.
The net removal rate per unit volume is then

\[
\frac{1}{A(x)} \frac{\partial \phi}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} [v(x,t) A(x) C(x,t)] , \quad \text{or}
\]

\[
\frac{1}{A(x)} \frac{\partial \phi}{\partial x} = v(x,t) \frac{\partial C(x,t)}{\partial x} + \left[ \frac{\partial v(x,t)}{\partial x} \frac{v(x,t)}{A(x)} + \frac{v(x,t)}{A(x)} \frac{dA(x)}{dx} \right] C(x,t) , \quad \text{atoms cm}^{-3}\cdot\text{sec}^{-1}.
\]

Collecting all source and removal terms, the rate equation for the fission product concentration in the coolant becomes

\[
\frac{\partial C(x,t)}{\partial t} = \dot{q}_c(x,t) + \frac{P(x)}{A(x)} h(x,t) [B(x,t) - C(x,t)]
\]

\[
- v(x,t) \frac{\partial C(x,t)}{\partial x} - \left[ \Lambda_s + \frac{\partial v(x,t)}{\partial x} + \frac{v(x,t)}{A(x)} \frac{dA(x)}{dx} \right] C(x,t) .
\]

Defining

\[
\Lambda_c(x,t) = \Lambda_s + \frac{\partial v(x,t)}{\partial x} + \frac{v(x,t)}{A(x)} \frac{dA(x)}{dx} \quad (3)
\]

as the effective decay constant for the coolant concentration, the rate equation can be written in a more compact form:

\[
\frac{\partial C(x,t)}{\partial t} = \dot{q}_c(x,t) + \frac{P(x)}{A(x)} h(x,t) [B(x,t) - C(x,t)]
\]

\[
- v(x,t) \frac{\partial C(x,t)}{\partial x} - \Lambda_c(x,t) C(x,t) .
\]

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3.3 THE COUPLED COOLANT-SURFACE EQUATION SYSTEM

Equations (2) and (4) for S and C are not sufficient for a complete description of the problem. An additional equation is needed to define the relationship between the boundary layer concentration B and the surface concentration S. Also, initial values for C and S must be specified, and a boundary condition for the inflowing coolant at the upstream end must be specified. The sign convention shown below is used to specify the flow directions.

\[ v > 0 \quad \rightarrow \quad v < 0 \]

\[ x = 0 \quad \rightarrow \quad x = L_b \quad \text{positive } x \text{ direction} \]

With the additional information the complete set of equations for a single branch is

\[
\begin{align*}
\frac{\partial C(x,t)}{\partial t} &= q_c(x,t) + \frac{p(x)}{A(x)} h(x,t) [B(x,t) - C(x,t)] - v(x,t) \frac{\partial C(x,t)}{\partial x} - A_c(x,t) C(x,t) \\
\frac{\partial S(x,t)}{\partial t} &= q_s(x,t) - h(x,t) [B(x,t) - C(x,t)] - A_s S(x,t)
\end{align*}
\]

(5)  (6)

\[ B(x,t) = f[S(x,t)]* \]

(7)

\[
\begin{align*}
C(x,0) &= C_0(x) \\
S(x,0) &= S_0(x)
\end{align*}
\]

(8)

\[
\begin{align*}
C(0,t) &= C_{x0}(t), \quad v > 0 \\
C(L_b,t) &= C_{xL}(t), \quad v < 0
\end{align*}
\]

(9)

*This functional relationship, valid for an assumed state of equilibrium, will be explained in more detail in the next section.
Several observations can be made about these equations:

- The coolant and surface concentrations are coupled via a mass transfer term that involves the difference between the boundary layer concentration $B$ and the bulk coolant concentration $C$.

- For $B > C$ this term is a removal rate for $S$ and a source rate for $C$. This condition is usually realized in the core coolant channels where the source rate $q_s > 0$. Outside the core $q_s$ is zero and the concentration $C$ picked up from the plateout surface in the core is larger than $B$. The coupling term reverses its sign and becomes a removal rate for the coolant concentration $C$ and a source rate for the plateout concentration $S$.

- The boundary condition is imposed at the upstream end of the branch. Mathematically, one could apply the boundary condition at the branch outlet. However, as was pointed out in Ref. 3, a downstream boundary condition would be physically meaningless.

3.3.1 The Sorption Equation

The sorption Eq. (7) is generally nonlinear. For example, in the case of a Freundlich sorption mechanism Eq. (7) becomes

$$B(x,t) = K(x,t) \ Y(x,t) \ S(x,t)^\gamma(x,t) \ , \ \gamma > 1 \ .$$

For this reason the system (5), (6) is generally a nonlinear system of partial differential equations. Because of this nonlinearity and the fact that most of the parameters are allowed to change with time and spatial position, a finite difference procedure is used to solve for $C$ and $S$. This procedure will be discussed in Section 4. For the present it will
be noted that in a finite difference formulation the problem reduces in
general to the solution of a system of simultaneous algebraic equations.
For the solution procedure to be efficient on a digital computer, it is
useful that these algebraic equations be linear. In the present analysis
the system will therefore be derived by linearizing the differential
equations. The nonlinear terms will be later accounted for by an iteration
procedure.

Expanding $B(S)$ as a Taylor series about the most recent (best available)
guess, $S_g$, one obtains

$$B(S) = B(S_g) + \left( \frac{dB}{dS} \right)_{S_g} (S - S_g) = \phi(S_g) + \psi(S_g) S \tag{10},$$

where

$$\psi(S_g) = \left( \frac{dB}{dS} \right)_{S_g}, \quad \phi(S_g) = B(S_g) - S_g \psi(S_g) \tag{11}.$$

It is clear that as the iteration converges $S_g$ will approach the true solu-
tion $S$ and the linearization will be exact. Thus, in deriving the finite
difference equations that follow, it will be assumed that the linearization

$$B(x,t) = \phi(x,t) + \psi(x,t) S(x,t) \tag{12}$$

is exact.
4. FINITE DIFFERENCE EQUATIONS

4.1 INTRODUCTION

With the aid of (12) the system of Eqs. (5) through (9) is now linear. Substituting (12) into Eqs. (5) and (6) one obtains the coupled linear differential equations

\[
\frac{3C(x,t)}{3t} = q_c(x,t) + \frac{F(x)}{A(x)} h(x,t) \left[ \phi(x,t) + \psi(x,t) S(x,t) - C(x,t) \right]
\]

\[ - \nu(x,t) \frac{3C(x,t)}{3x} - \Lambda_c(x,t) C(x,t) \]

\[ \equiv F \left[ x, t, S(x,t), C(x,t), \frac{3C(x,t)}{3x} \right], \quad (13) \]

\[
\frac{3S(x,t)}{3t} = q_s(x,t) - h(x,t) \left[ \phi(x,t) + \psi(x,t) S(x,t) - C(x,t) \right]
\]

\[ - \Lambda_s S(x,t) \equiv G \left[ x, t, S(x,t), C(x,t) \right]. \quad (14) \]

The functions F and G are a shorthand notation for "everything on the right side." These functions are used later in describing an implicit time integration scheme.

We shall now proceed to discretize this system of differential equations by applying finite difference approximations in time and space.
4.2 DISCRETIZATION OF TIME

We divide the integration time interval $t_L - t_0$ into small time steps
$
\Delta t_k = t_k - t_{k-1}
$
as shown in the sketch.

If we have a first-order differential equation of the form

$$
\frac{\partial y(x,t)}{\partial t} = z(x,t,y),
$$

we can formally integrate between $t_{k-1}$ and $t_k$ and arrive at

$$
y(x,t_k) = y(x,t_{k-1}) + \int_{t_{k-1}}^{t_k} z(x,t,y) \, dt = y(x,t_{k-1}) + \overline{z}(x)(t_k - t_{k-1}).
$$

The term $\overline{z}$ is the time average value of $z(x,t,y)$ between $t_{k-1}$ and $t_k$.

If we now assume $z$ to be monotonically increasing or decreasing in $\Delta t_k$, and if we further assume that the spatial shape of $z$ is independent of time in $\Delta t_k$, then there exists a value of the time integration parameter $\theta$ in the interval $0 < \theta < 1$ such that

$$
\overline{z} = (1-\theta) z_{k-1} + \theta z_k, \quad t_{k-1} \leq t \leq t_k.
$$

In Eq. (17) we have introduced the simpler notation $z^\ell \equiv z[x,t^\ell,y(x,t^\ell)]$ to be used in all future developments.
For any given value of $x$ there is one value of $\theta$ for which (17) is exact, as illustrated below.

For example, if $\theta$ is taken to be zero, then $\bar{z} \approx z^{l-1}$. For $\theta = 1$, $\bar{z} \approx z^l$.

If $z$ were a linear function of $t$ in $\Delta t^l$, $\theta = \frac{1}{2}$ would be exact. In our case, since $z$ is a function of both $x$ and $t$, the assumption of constant $\theta$ in Eq. (17) is an approximation.

Inserting (17) into (16) yields

$$y^l = y^{l-1} + [(1-\theta) z^{l-1} + \theta z^l] (\Delta t^l).$$

This is a recursive formula for marching forward in time, successively solving for $y^l$ as a function of $y^{l-1}$. Depending on $\theta$ this integration scheme is known as

- fully explicit, $\theta = 0$
- Crank Nicholson, $\theta = \frac{1}{2}$, and
- fully implicit, $\theta = 1$. 

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The time integration procedure described for the general Eq. (15) will now be used to integrate the equations for the coolant and plateout concentrations over the time interval $\Delta t^t$. From (13) and (14) we obtain then

$$C^t = C^{t-1} + \left[ (1-\theta) F^{t-1} + \theta F^t \right] \Delta t^t, \quad (19)$$

$$S^t = S^{t-1} + \left[ (1-\theta) G^{t-1} + \theta G^t \right] \Delta t^t. \quad (20)$$

Solution of the coupled system (19) and (20) can be achieved by eliminating $S^t$ in favor of $C^t$ and deriving a single matrix equation with $C^t(x)$ as the only unknown. As a first step we substitute the explicit form of $G$ from Eq. (14) into Eq. (20). Rearranging terms to solve for $S^t$, the result is

$$S^t = \frac{\left\{ (1-\theta) \left[ h^{t-1}(C^{t-1} - \phi^{t-1}) + q_s \right] + \theta \left[ h^t (C^t - \phi^t) + q_s \right] \right\} \Delta t^t}{1 + \theta \Delta t^t (h^t \psi^t + \Lambda_s)} \quad (21)$$

where except for $\Lambda_s$, $\theta$ and $\Delta t^t$, all variables depend on $x$. Eq. (21) will later be used to compute $S^t$ from known values of $S^{t-1}$, $C^{t-1}$ and $C^t$. For the present we will use it to eliminate $S^t$ from the $F^t$ term in Eq. (19), whereby $S^t$ from Eq. (21) is substituted into the explicit function $F^t$ from Eq. (13). The resulting expression for $F^t$, which no longer contains $S^t$, is then substituted into Eq. (19). The terms can then be rearranged such that the unknowns at time point $t=t^t$ are on the left and the known values for $t=t^t-1$ on the right. The final result, after some manipulation, is
\[(1 + \theta \Delta t_x a^l) C^l + \theta \Delta t_x \nabla \frac{\partial C^l}{\partial x} =\]
\[
\left[1 - (1-\theta)\Delta t_x \beta^{l-1,l}\right] C^{l-1} - (1-\theta)\Delta t_x \nabla^{l-1} \frac{\partial C^{l-1}}{\partial x} + y^{l-1,l},
\]

where
\[
\alpha^l \equiv \Lambda^l_c + \frac{P}{A} h^l - \frac{\theta \Delta t_x \frac{P}{A} (h^l)^2 \psi}{1 + \theta \Delta t_x (h^l \psi + \Lambda_s)},
\]
\[
\beta^{l-1,l} \equiv \Lambda^{l-1}_c + \frac{P}{A} h^{l-1} - \frac{\theta \Delta t_x \frac{P}{A} h^{l-1} \psi^l}{1 + \theta \Delta t_x (h^l \psi^l + \Lambda_s)},
\]
\[
y^{l-1,l} \equiv (1-\theta) \Delta t_x \gamma^{l-1} + \theta \Delta t_x (\delta^l + \omega^{l-1,l}),
\]

and where \(\gamma, \delta, \text{ and } \omega\) in (25) are given by
\[
\gamma^{l-1} \equiv \frac{P}{A} h^{l-1} (\phi^{l-1} + \psi^{l-1} S^{l-1}) + \phi^l_c,
\]
\[
\delta^l \equiv \frac{P}{A} h^l \phi^l + \phi^l_c, \quad \text{and}
\]
\[
\omega^{l-1,l} \equiv \frac{P}{A} h^l \psi^l \left[1 - (1-\theta)\Delta t_x (h^l \psi^l + \Lambda_s)\right] S^{l-1} - \frac{1 + \theta \Delta t_x (h^l \psi^l + \Lambda_s)}{
\left[1 + \theta \Delta t_x (h^l \psi^l + \Lambda_s)\right] \left[1 + \theta \Delta t_x (h^l \psi^l + \Lambda_s)\right]}
\]
\[
\left[(1-\theta)(q_s^{l-1} - h^{l-1} \phi^{l-1}) + \theta (q_s^{l-1} \phi^l)ight] \Delta t_x
\]
4.3 SPATIAL DISCRETIZATION

Equation (22) contains only the unknowns \( C' \) and \( \partial C'/\partial x \). In order to be able to solve for \( C'(x) \) we have to discretize spatially and approximate \( \partial C'/\partial x \) by finite differences. For reasons of accuracy, central differences are the obvious choice. However, for the particular problem on hand, it turns out that forward or backward differences are more appropriate to avoid singularities of the system matrix. This was extensively discussed in Ref. 3.

Consider now the sketch showing the branch length \( L_b \) divided into \( n-1 \) increments of length \( \Delta x_k = x_{k+1} - x_k \).

Instead of Eq. (22) for a general \( x \) we will employ one finite difference equation for each of the spatial positions \( x_1 \) to \( x_n \). Depending on which end of the branch is the coolant inlet (\( x=x_1 \) or \( x=x_n \)) the first or the last of these \( n \) equations will be an expression for the boundary condition. The method for determining this boundary condition (when it is not given explicitly as a global boundary condition) will be discussed in Section 5. For the moment we shall derive the typical difference equations only for the nodal points \( x_2 \) to \( x_n \) (for positive coolant velocities) and \( x_1 \) to \( x_{n-1} \) (for negative velocities). For \( v>0 \), \( \partial C/\partial x \) will be approximated by backward differences and for \( v<0 \) by forward differences.
Consider first backward differences* ($v > 0$):

\[
\frac{\partial C}{\partial x}\bigg|_{x=x_k} = \frac{C_k - C_{k-1}}{\Delta x_{k-1}} = -\frac{1}{\Delta x_{k-1}} C_{k-1} + \frac{1}{\Delta x_{k-1}} C_k , \quad 2 \leq k \leq n . \quad (29)
\]

We now define the coefficients

\[
\alpha_k^{l-1} = \left(1 - \frac{v}{\Delta x_{k-1}}\right) , \quad \beta_k^{l-1} = \frac{v}{\Delta x_{k-1}} ,
\]

\[
\alpha_k^l = \alpha_k^{l-1} + \frac{v_k}{\Delta x_{k-1}^{l-1}} , \quad \beta_k^l = \beta_k^{l-1} + \frac{v_k}{\Delta x_{k-1}^{l-1}} , \quad (30)
\]

and introduce them into Eq. (22) for $x_2$ to $x_n$. Eq. (22) then becomes

\[
C_k^l + \Delta t_l \left(\alpha_k^{l-1} C_{k-1} + \alpha_k^l C_k\right) = \]

\[
= C_k^{l-1} - (1-\varepsilon) \Delta t_l \left(\beta_k^{l-1} C_{k-1} + \beta_k^l C_k\right) + y_k^{l-1} , \quad (31)
\]

\[
2 \leq k \leq n
\]

* In what follows we introduce the notation $f(x_k) \equiv f_k$. 

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With the \((n-1) \times n\) matrices:

\[
\left[ \begin{array}{c} 1 \end{array} \right]_{(n-1) \times n}, \quad A^t = \left[ \begin{array}{ccc} a_{21} & a_{22} \\ \vdots & \ddots & \ddots \\ a_{n-2,n-1} & a_{n-1,n} & a_{n,n} \end{array} \right]_{(n-1) \times n}
\]

\[
\left[ \begin{array}{c} d_{21} \\ d_{22} \\ \vdots \\ d_{n-1,n} \end{array} \right]_{(n-1) \times n}
\]

\[D_{b}^{t-1,t} = \left[ \begin{array}{ccc} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \\ c_n \end{array} \right]_{n \times 1}, \quad (y_{b})^{t-1,t} = \left[ \begin{array}{c} y_2 \\ y_3 \\ \vdots \\ y_{n-1} \\ y_n \end{array} \right]_{(n-1) \times 1}
\]

* The index \(b\) stands for backward differences.
the n-1 equations of system (31) can be represented in matrix notation in the form

\[
\begin{bmatrix}
I_b + \theta \Delta t^k A^t
\end{bmatrix} \xi^t = \begin{bmatrix}
I_b - (1-\theta) \Delta t^k D^{-1, t}^l
\end{bmatrix} \xi^{t-1} + \left( \Omega^{t-1, t} \right)_b \quad (34)
\]

If we call the right hand side of (34) the (n-1) x 1 "force vector" \( (\Omega^{t-1, t})_b \), the system of equations for the nodal points \( x_2 \) to \( x_n \) can finally be written as

\[
\begin{bmatrix}
I_b + \theta \Delta t^k A^t
\end{bmatrix} \xi^t = \left( \Omega^{t-1, t} \right)_b , \quad v_k^t > 0 \quad . \quad (35)
\]

From (35), the significance of the value of \( \theta \) in terms of the time integration is now quite clear. With the boundary condition \( C_1^t \) given as first equation, \( \theta=0 \) yields \( C_k^t \) explicitly as \( C_k^t = (\Omega_{k}^{t-1, t})_b \), \( k > 1 \). For \( \theta=1 \), \( C_k^t \), \( k > 1 \) is given implicitly.

We now turn to negative velocities for which a similar matrix equation can be derived. Since the coolant enters the branch at \( x=x_n \), the nth equation will be the boundary condition and we consider here only the first n-1 equations.

The forward differences are

\[
\frac{\partial C}{\partial x} \bigg|_{x=x_k^{t-1}} = \frac{C_{k+1}^t - C_k^t}{\Delta x_k} = \frac{1}{\Delta x_k} C_k + \frac{1}{\Delta x_k} C_{k+1}^t , \quad 1 \leq k \leq n-1 \quad . \quad (36)
\]
Defining now coefficients analogous to $a$ and $d$,

\[
\begin{align*}
    u_{k,k}^{l} &= a_{k}^{l} - \frac{v_{k}^{l}}{\Delta x_{k}^{l}} \\
    w_{k,k}^{l-1} &= b_{k}^{l-1} - \frac{v_{k}^{l-1}}{\Delta x_{k}^{l}} \\
    u_{k,k+1}^{l} &= \frac{v_{k}^{l}}{\Delta x_{k}^{l}} \\
    w_{k,k+1}^{l-1} &= \frac{v_{k}^{l-1}}{\Delta x_{k}^{l}}
\end{align*}
\]

the equivalent of Eq. (31) is

\[
\begin{align*}
    C_{k}^{l} + 6 \Delta t \left( u_{k,k}^{l} C_{k}^{l} + u_{k,k+1}^{l} C_{k+1}^{l} \right) &= \\
    = C_{k}^{l-1} - (1-\theta) \Delta t \left( w_{k,k}^{l-1} C_{k}^{l-1} + w_{k,k+1}^{l-1} C_{k+1}^{l-1} \right) + y_{k}^{l-1,1} \\
    1 \leq k \leq n-1.
\end{align*}
\]

With the matrices*

\[
I_{f}^{l} = \begin{bmatrix}
    1 & & & & & \\
    & 1 & & & & \\
    & & \ddots & & & \\
    & & & 1 & & \\
    & & & & \ddots & \\
    & & & & & \ddots
\end{bmatrix}_{(n-1) \times n}, \quad
U_{f}^{l} = \begin{bmatrix}
    u_{11} & u_{12} & & & & \\
    u_{22} & u_{23} & & & & \\
    & & \ddots & & & \\
    & & & u_{n-2,n-1} & & \\
    & & & & u_{n-2,1} & \\
    & & & & & u_{n-1,n-1}
\end{bmatrix}_{(n-1) \times n}
\]

(Continued)

* The index $f$ stands for forward differences.
and vectors

\[
\begin{bmatrix}
C_1 \\
C_2 \\
\vdots \\
C_{n-1} \\
C_n
\end{bmatrix}^{(n-1)\times 1}
\]

\[
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_{n-1}
\end{bmatrix}^{(n-1)\times 1}
\]

Eqs. (38) can be written as

\[
\begin{bmatrix}
I_f + \theta \Delta t \frac{U_f^t}{C} \\
\end{bmatrix}^{(n-1)\times 1}
\]

\[
\begin{bmatrix}
I_f - (1-\theta) \Delta t \frac{W^{t-1}}{C} \\
\end{bmatrix}^{(n-1)\times 1} = \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f} + \left(\begin{bmatrix}
y_{t-1}^{f-1} \\
y_{t-1}^{f-1} \\
\vdots \\
y_{t-1}^{f-1}
\end{bmatrix}^{(n-1)\times 1} \right)_{f} \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f}, \tag{41}
\]

or

\[
\begin{bmatrix}
I_f + \theta \Delta t \frac{U_f^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f} = \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f} \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f} \left(\begin{bmatrix}
\frac{v_{t-1}^t}{C} \\
\end{bmatrix}^{(n-1)\times 1} \right)_{f}, \tag{42}
\]

\[\text{s.t. } v_{k}^{t} < 0.\]
Each of the equations (35) and (42) is a system of \( n - 1 \) equations in \( n \) unknown coolant concentrations \( C_1^t \) to \( C_n^t \). For a unique solution an additional equation representing the branch boundary condition is required. The complete \( n \times n \) systems are then

\[
\begin{align*}
C_1^t &= C_1^t(x=0) \\
\left[ I_b + \Theta \Delta t \Lambda \right] C^t &= \left( \Omega^{t-1} \right)_b \\
\end{align*}
\]

or

\[
\begin{align*}
\left[ I_f + \Theta \Delta t \Lambda \right] C^t &= \left( \Omega^{t-1} \right)_f \\
C_n^t &= C_n^t(x=L_b) \\
\end{align*}
\]

Having thus obtained a complete \( n \times n \) system (43), the incremental solution procedure for a linear relationship between the boundary layer concentration \( B \) and surface concentration \( S \) is straightforward. At \( t=t_0 \) the initial value conditions \( \bar{C}_0 \) and \( \bar{S}_0 \) are given and (43) can be solved for \( \bar{C}_1 \) at \( t = t_1 = t_0 + \Delta t_1 \). With \( \bar{C}_1 \) known, \( \bar{S}_1 \) can then be obtained from Eq. (21). The vector pair \( \bar{C}_1 \) and \( \bar{S}_1 \) are the initial value conditions for the second time step \( \Delta t_2 = t_2 - t_1 \), etc.

If \( B \) is nonlinear in \( S \), then a Newton-Raphson iterative procedure is used for the solution. At each stage \( i \) of the iteration one expands the nonlinear function \( B(S) \) as a linear approximation about the current guess \( S_{gi} \), i.e.,

\[
B_i(S) \approx \phi_i(S_{gi}) + \psi_i(S_{gi}) S_1.
\]

The system equations are assembled and solved assuming this linear relationship is exact, and the solution \( \bar{S} \) is projected to another improved guess. The iteration converges rapidly whenever the function \( B(S) \) is monotonic, as is the case in this analysis.
So far we have assumed that the branch boundary condition is known. However, this is only the case if the upstream branch end is a free end. Then the free end boundary condition is a global boundary condition. In the case that the upstream end of a branch is connected to any other branch, the incoming impurity flow rate is not explicitly known and has to be determined. The developments in connection with these unknown boundary conditions will be discussed in the following section.
5. BRANCH SYSTEM REDUCTION AND GLOBAL SYSTEM

5.1 INTRODUCTION

Consider, as an example, the following simple network of 5 branches with coolant mass flow rates \( \dot{m} \) (g He/sec). This network has 5 global nodal points. Only global point 1 is a free upstream branch end. There

\[
\begin{align*}
\text{BRANCH} & \quad \text{GLOBAL POINT 3} \\
1 & \quad 2 \quad 3 \\
\dot{m}_3 & \quad \dot{m}_2 \quad \dot{m}_1 \\
2 & \quad 4 \\
\dot{m}_1 & \quad \dot{m}_4 = \dot{m}_2 \\
3 & \quad 4 \\
\dot{m}_4 & \quad \dot{m}_5 \\
4 & \quad 5 \\
\dot{m}_5 & \quad (= \dot{m}_1 + \dot{m}_4)
\end{align*}
\]

an explicit global boundary condition has to be imposed on the network. Given this boundary condition one could solve system (43) for branch 3 and obtain the fission product flowrate at the downstream end node. If we now assume perfect gas mixing, the fission product flow rate of the downstream node of branch 3 will be apportioned to the inlets of branches 1 and 2 according to their coolant mass flow rates (mixing condition). The boundary conditions for branches 1 and 2 are now known. One could proceed and solve for the downstream end impurity flow rates of branches 1 and 2. At global point 3 we have continuity of impurity flow rates. The solution for the downstream end of branch 2 is thus the boundary condition for the upstream node of branch 4. The sum of the downstream impurity flow rates of branches 1 and 4 is the
boundary condition for branch \( \mathbf{5} \) at global point 4. With this known boundary condition, the solution for branch \( \mathbf{5} \) can finally be obtained.

It should be noted that this example is a "trivial" problem to solve because, by choosing the right order of evaluation, the solution in all branches can be found sequentially. In many practical problems, such as the HTGR loop geometries of Figures 3 and 4, the flow downstream of a given node will loop back and influence the boundary condition at the given node. Thus, in these cases the boundary conditions cannot be found sequentially, but they must be found by the solution of a set of simultaneous equations for the global network. For this reason PADLOC organizes the global network equations in a very general manner and employs the simultaneous solution technique rather than attempting to find a sequential path.

It is clear that we need to determine all boundary conditions before proceeding to solve for interior branch nodes. One can accomplish this by reducing each branch equation system to a single relationship between inlet and outlet fission product flow rates. These equations coupled with explicitly given global boundary conditions at free upstream branch ends and mixing equations at branch connections will then constitute a global equation system for the unknown impurity flow rates at branch ends. After solving the global system, one can then proceed to obtain the solution for the interior branch nodes. The first step in establishing the global system of equations is therefore the reduction of the equation system of a single branch. This we will discuss in the following section.

5.2 REDUCTION OF THE EQUATION SYSTEM OF A SINGLE BRANCH

Consider the system (35) for positive flow velocities:

\[
\begin{bmatrix}
I_b + \theta \Delta t \ A^k \\
\end{bmatrix}
\mathbf{c}^t = \left( \frac{\mathbf{c}^{t-1}}{\Omega} \right)_b.
\]
We first simplify notation by introducing

\[ B = I_b + \theta \Delta t_b A^b \]  \hspace{1cm} (44)

and

\[ \hat{H} = \left( \hat{C}^{t-1, t} \right)_b \] \hspace{1cm} (45)

If we also omit the time index \( t \) from \( \hat{C}^t \), we obtain

\[ B \hat{C} = \hat{H} \] \hspace{1cm} (46)

Here,

\[ B = \begin{bmatrix}
  b_{21} & b_{22} \\
  b_{32} & b_{33} \\
  & \ddots \\
  & & b \\
  & & b \\
  & & & b_{n,n} \\
  & & & b_{n,n-1} \\
  & & & & & b_{n-2,n-1} \\
  & & & & & & b_{n-1,n-1} \\
  & & & & & & & b_{n-1,n-1} \\
  & & & & & & & & b \\
  & & & & & & & & b \\
  & & & & & & & & & & b_{n-1,n} \\
  & & & & & & & & & & & & b_{n,n} \\
\end{bmatrix}_{(n-1) \times n} \]

\[ \hat{C} = \begin{bmatrix}
  c_1 \\
  c_2 \\
  c_3 \\
  \cdot \\
  c_{n-1} \\
  c_n \\
\end{bmatrix}_{n \times 1} \]

\[ \hat{H} = \begin{bmatrix}
  H_2 \\
  H_3 \\
  \cdot \\
  H_{n-1} \\
  H_n \\
\end{bmatrix}_{(n-1) \times 1} \]
We can partition $B$ into submatrices and the vectors into subvectors as shown below.

\[
\begin{bmatrix}
  b_{21} & b_{22} \\
  b_{32} & b_{33} \\
  \vdots & \vdots \\
  b_{n-1,n-1} & b_{n-1,n} \\
  b_{n,n-1} & b_{n,n}
\end{bmatrix}
\begin{bmatrix}
  c_1 \\
  c_2 \\
  c_3 \\
  \vdots \\
  c_{n-1} \\
  c_n
\end{bmatrix}
= \begin{bmatrix}
  H_2 \\
  H_3 \\
  \vdots \\
  H_{n-1} \\
  H_n
\end{bmatrix}
\]

Here, we introduced the index $i$ for the subvectors $\hat{c}_i$ and $\hat{H}_i$ relating to interior nodes. The definition of $B_{im}$ is obvious from the partitioning.

Writing out the partitioned equation we obtain

\[
B_{21}c_1 + B_{22} \hat{c}_1 = H_1 
\]

\[
B_{32} \hat{c}_1 + B_{33}c_n = H_n. 
\]

From (47),

\[
\hat{c}_1 = B_{22}^{-1}\left(\hat{H}_1 - B_{21}c_1\right). 
\]
Substituting (49) into (48) eliminates $\bar{C}_1$, giving one equation in two unknowns:

$$- B_{32}^{-1} B_{21} B_{22} C_1 + B_{33} C_n = H_n - B_{32}^{-1} B_{22}^{-1} \hat{H}_1 .$$  

Equation (50) is the reduced branch equation relating branch end concentrations $C_1$ and $C_n$.

In order to combine equations of the form (50) with appropriate mixing equations (for the purpose of establishing the global equation system) it is useful to consider fission product flow rates $\dot{M}$ instead of concentrations $C$.

With $v$ being the velocity and $A$ the conduit cross section area, the atom flow rate at branch nodal point $k$ is

$$\dot{M}_k = A_k v_k C_k , \frac{\text{atoms}}{\text{sec}} .$$  

We now transform Eq. (50) by multiplying both sides by the product $A_1 v_1 A_n v_n$. The result is

$$B_{11}^* \dot{M}_1 + B_{nn}^* \dot{M}_n = H^* ,$$  

where

$$B_{11}^* \equiv - A_1 v_1 B_{32} B_{22}^{-1} B_{21} ,$$  

$$B_{nn}^* \equiv A_1 v_1 B_{33} , \text{ and}$$  

$$H^* \equiv A_1 v_1 A_n v_n \left( H_n - B_{32} B_{22}^{-1} \hat{H}_1 \right) .$$
For \( v<0 \), the developments are similar. Defining
\[
E = I_f + \theta \Delta t \mu^t, \\
\hat{R} = \left( \hat{\mu}^{t-1}, t \right)_f,
\]
Eq. (42) becomes
\[
E \hat{C} = \hat{R}. \tag{54}
\]
This matrix equation can be partitioned as shown below

\[
\begin{bmatrix}
 e_{11} & e_{12} \\
 e_{22} & e_{23}
\end{bmatrix}
\begin{bmatrix}
 C_1 \\
 C_2 \\
 \vdots \\
 C_{n-2} \\
 C_{n-1} \\
 C_n
\end{bmatrix}
= \begin{bmatrix}
 R_1 \\
 R_2 \\
 \vdots \\
 R_{n-2} \\
 R_{n-1} \\
 C_n
\end{bmatrix},
\]

or,
\[
\begin{bmatrix}
 E_{11} & E_{12} & 0 \\
 0 & E_{22} & E_{23}
\end{bmatrix}
\begin{bmatrix}
 C_1 \\
 \hat{C}_1 \\
 C_n
\end{bmatrix}
= \begin{bmatrix}
 R_1 \\
 \hat{R}_1 \\
 C_n
\end{bmatrix}.
\]

38
From

\[
E_{22} \dot{C}_1 + E_{23} C_n = \dot{R}_1 ,
\]

follows

\[
\dot{C}_1 = E_{22}^{-1} \left( \dot{R}_1 - E_{23} C_n \right) ,
\]

and the reduced equation is

\[
E_{11}^* \dot{M}_1 + E_{nn}^* \dot{M}_n = R^* .
\]

Here

\[
E_{11}^* \equiv A_n v_n E_{11}
\]

\[
E_{nn}^* \equiv - A_1 v_1 E_{12} E_{22}^{-1} E_{23}
\]

\[
R^* \equiv A_1 v_1 A_n v_n \left( R_1 - E_{12} E_{22}^{-1} R_1 \right) .
\]

Equations (49) for \( v > 0 \) and (55) for \( v < 0 \) relate the concentrations of the interior branch nodes to the boundary concentrations \( C_1 \) or \( C_n \). These equations are later used to obtain the interior solution. At the moment, however, we consider the reduced equations together with global conditions and mixing equations to set up the global system.

5.3 MIXING EQUATIONS

As mentioned before, for any upstream branch end at which no global boundary condition is imposed, we need to determine the branch boundary condition. Such a boundary condition is given implicitly by the mixing equation for the upstream global nodal point. Consider a global node with several branches connected to it.
Incoming branches are branches whose coolant flow directions are towards the connecting global point. For outgoing branches the flow directions are away from the global node. The incoming branch end impurity flow rates at nodes $n$ are designated $(\dot{M}_n)_i$ and the fission product flow rates at the first node of the outgoing branches are $(\dot{M}_1)_j$; $m_j$ are the coolant mass flow rates in the outgoing branches. If we now assume perfect mixing at the connection point, the impurity mass concentrations in all outgoing branches are the same. Then the impurity flow rates will be apportioned according to the coolant mass flow rates, or,

\[
(\dot{M}_1)_j = \frac{m_j}{\sum m_j} \sum_j (\dot{M}_1)_j ,
\]

where $j$ is a particular value of $j$.

Considering conservation of flow rates at the connection,

\[
\sum_i (\dot{M}_n)_i = \sum_{j \neq i} (\dot{M}_1)_j ,
\]
Eq. (58) becomes

\[
\frac{\dot{M}_1}{j} = \frac{m_j}{m_j} \sum_{i \neq j} (\hat{M}_n)_i .
\] (59)

This is the auxiliary mixing equation for the outgoing branch \(j\).

Three special cases can be considered:

a. global point with only outgoing branches:

In this case the global point contains only free upstream branch ends and a global boundary condition has to be imposed at \(g\). If the incoming flow rate is \(\dot{M}_g\), then we have

\[
(\hat{M}_1)_j = \frac{m_j}{m_j} \dot{M}_g .
\] (60)

instead of (59).

b. global point with several incoming and only one outgoing branch:
Equation (59) for this case is simply
\[ (\dot{M}_j)_j = \sum_i (\dot{M}_n)_i \]  \hspace{1cm} (61)

c. continuity:

Here we have only one incoming and one outgoing branch

and Eq. (61) reduces to
\[ (\dot{M}_j)_j = (\dot{M}_n)_i \]  \hspace{1cm} (62)

This is really a superfluous equation since it can be avoided by a proper numbering of the global unknowns. This will become clear in the following section where the assembly of the global equations will be shown.

It is noted that the coolant and plateout concentrations are in general discontinuous at branch interfaces. Consider two branches of lengths \( L_1 \) and \( L_2 \) and coolant mass flow rates \( \dot{m} \) in series:

At the junction the impurity flow rates are continuous, so
\[ \dot{M}_1(L_1) = \dot{M}_2(0) \]
This gives for the coolant concentrations (A is the cross section area)

\[ C_2(0) = \frac{A_1(L_1) v_1(L_1)}{A_2(0) v_2(0)} C_1(L_1) \]

Now the velocities in the above equation can be related to coolant pressure and coolant temperature via the coolant density, the coolant mass flow rate, and the ideal gas law:

\[ v = \frac{m}{Ap} \cdot \]

Because of the fact that the temperatures at a junction are continuous,

\[ \frac{A_1(L_1) v_1(L_1)}{A_2(0) v_2(0)} = \frac{p_2(0)}{p_1(L_1)} \]

thus

\[ C_2(0) = \frac{p_2(0)}{p_1(L_1)} C_1(L_1) \]

If there are no area discontinuities in the channel, then \( p_2(0) = p_1(L_1) \), and the coolant concentrations are continuous. However, for an orifice or for an abrupt change in area there may be a pressure drop at the junction, and the coolant concentrations can be discontinuous. The pressures at both branch ends are independently specified by the PADLOC user, so the program automatically accounts for this.

In the case of the surface concentration, the sorption characteristics depend on the branch material (graphite, steel, etc.). In addition, the surface source rates may differ from branch to branch (core, portions outside the core). Thus, the surface concentration is generally discontinuous at branch interfaces.
This section describes how the equations for individual branches, including the mixing and boundary conditions, are combined (assembled) to form a global system of equations for the network as a whole. In the PADLOC program there is a logical procedure whereby the unknown impurity mass flows are ordered as the assembly progresses. The number and the order of the unknowns can vary with time whenever the directions of the mass flows are changed. For the sake of brevity the details of this logic will be omitted, and we will present the assembly procedure by means of a typical example in which the direction of the flows are assumed, and the unknowns are already numbered. In this example we will assemble the equations for the network previously discussed in Section 5.1. For convenience the sketch has been redrawn (see following page) to show more detail. It is assumed that all mass flows are positive in the direction of the arrows. A convention for defining this through user input will be explained later.

The square boxes in the sketch represent the global points and the \( X_i \) within the boxes are the 9 unknown branch end impurity flow rates. With the exception of branch 4 we will need two equations for each branch. The first equation is either a global boundary condition or a mixing equation. The second equation is the reduced branch equation (52). The first equation for branch 4 would be the continuity condition (62), but this is eliminated by denoting \( X_3 \) as both the downstream unknown for branch 2 and the upstream unknown for branch 4. We start the assembly with the equations for branch 1 and proceed sequentially to branch 5. The final set of equations is shown on page 46 following the sketch.
\[
\begin{align*}
X_7 - \alpha_{12} X_2 &= 0, \quad \alpha_{12} = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2} \quad \text{(mixing)} \\
(B_{11})_1 X_7 + (B_{nn})_1 X_8 &= (H^*)_1 \quad \text{(reduced equation)} \\
X_6 - \alpha_{32} X_2 &= 0, \quad \alpha_{32} = \frac{\dot{m}_2}{\dot{m}_1 + \dot{m}_2} \quad \text{(mixing)} \\
(B_{11})_2 X_6 + (B_{nn})_2 X_3 &= (H^*)_2 \quad \text{(reduced equation)} \\
X_1 &= z_1 \quad \text{(global boundary condition at point 1)} \\
(B_{11})_3 X_1 + (B_{nn})_3 X_2 &= (H^*)_3 \quad \text{(reduced equation)} \\
(B_{11})_4 X_3 + (B_{nn})_4 X_9 &= (H^*)_4 \quad \text{(reduced equation)} \\
X_4 - X_8 - X_9 &= 0 \quad \text{(mixing)} \\
(B_{11})_5 X_4 + (B_{nn})_5 X_5 &= (H^*)_5 \quad \text{(reduced equation)}
\end{align*}
\]

Note: The additional index \(i\) in \((B_{kk}^*)_i\) and \((H^*)_i\) is the branch index.
The equivalent matrix equation is

\[
\begin{array}{cccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
-a_{12} & -a_{13} & (B^*_{11}) & & & (B^*_{nn}) & & & & \\
& -a_{22} & 1 & (B^*_{22}) & & & & & & \\
& & & -a_{32} & 1 & (B^*_{32}) & & & & \\
& & & & & (B^*_{nn}) & & & & \\
1 & & & & & & (B^*_{11}) & & & \\
& & & & & & & (B^*_{nn}) & & & \\
& & & & & & & & (B^*_{nn}) & & \\
& & & & & & & & & 1 & (B^*_{nn}) \\
& & & & & & & & & -1 & -1 \\
& & & & & & & & & (B^*_{nn}) & & \\
\end{array}
\]

\[
\begin{bmatrix}
X_1 \\
X_2 \\
X_3 \\
X_4 \\
X_5 \\
X_6 \\
X_7 \\
X_8 \\
X_9
\end{bmatrix} =
\begin{bmatrix}
0 \\
(H^*)_1 \\
0 \\
(H^*)_2 \\
Z_1 \\
(H^*)_3 \\
(H^*)_4 \\
0 \\
(H^*)_5
\end{bmatrix}
\]
We can now solve the global system (63), transform back to concentrations

\[
\begin{align*}
(C_1)_{1} &= \frac{1}{(A_1 v_1)_{1}} x_1 \\
(C_n)_{1} &= \frac{1}{(A_n v_n)_{1}} x_1 \\
\text{etc.} &- - - - - - - - - - \\
(C_1)_{5} &= \frac{1}{(A_1 v_1)_{5}} x_4 \\
(C_n)_{5} &= \frac{1}{(A_n v_n)_{5}} x_5
\end{align*}
\]

and use Eq. (49) to solve for the concentrations \( \hat{C}_i \) of the interior branch nodes. With \( \hat{C} \) now known, we compute \( \hat{S} \) from Eq. (21).

The assembly procedure illustrated here is handled automatically for an arbitrary network by the PADLOC code. The logic is too complicated to present in detail here. In essence, the procedure involves searching the branches in numerical order and allocating a unique index (e.g., 1 through 9) to the unknown mass flows at each end node. Repeated unknowns are omitted. The index allocation is repeated any time a flow changes direction because flow reversals can affect the ordering and the number of unknowns.

5.5 NEGATIVE FLOWS

PADLOC can handle both positive and negative flows. For example, flow reversals may be encountered whenever there is a transition from forced to natural convection, or vice versa. As previously mentioned, flow reversals can change the number and the order of the unknowns. Another complication involving the sign of the unknown might also occur in some circumstances. This section explains the nature of that complication by means of an example.
Consider the branches defined so that their positive directions, hence positive flow directions, converge on a single node, as shown below.

Although it is physically improbable that flows will actually be directed in this manner, the network description is arbitrary, so this case is admissible. Suppose the coolant flow in branch 2 is reversed, i.e., defined so that $\dot{m}_2$ is negative, as shown below.

Now the physically valid solution for the impurity flow rates at node A is $(\mathcal{M}_1)_A = -(\mathcal{M}_2)_A$. This is inconsistent with the assumed continuity condition, Eq.(62), in which the flow rates must be equal. The elimination of the unknown $(\mathcal{M}_2)_A$ by means of Eq.(62) is possible only by redefining the global equations in terms of the absolute values of the unknowns, maintaining a separate sign flag as an additional variable. For this reason, whenever a branch with negative flow is encountered, the sign of $R^*$ is changed in Eq.(56), and, if a global boundary condition is specified, its sign is changed as well. This measure guarantees that the solution of the global system is in terms of absolute values. Before returning to solve for interior branch concentrations, the branch end impurity flow rates of branches with negative coolant flows are changed back to their physically correct negative values.
6. USER'S MANUAL

6.1 INTRODUCTION TO PADLOC CAPABILITIES

PADLOC is designed to calculate the coolant and plateout concentrations of a single decaying fission product carried by the coolant through a network of pipes (branches). The code is variably dimensioned, and, with an extended core of 165,000 words, it allows a maximum problem size of \((\text{branches}) \times (\text{nodes per branch}) \approx 13,000\). All parameters that physically may depend on time and spatial position are recognized by the code as such. Some useful features that make PADLOC applicable to a variety of problems are as follows:

1. The flow geometry is idealized as an arbitrary network. Coolant mass flow rates are branch- and time-dependent. Flow reversals and zero flows are permitted.

2. One can choose a time integration scheme ranging from fully explicit to fully implicit. With the fully implicit option \((\theta = 1)\) large time steps can be employed in a quasi-steady-state analysis. Smaller time steps and \(\theta = \frac{1}{2}\) are appropriate for capturing transients.

3. Four options for branch dependent sorption behavior are provided. These describe the relationship between the coolant boundary layer concentration \(B(\text{atoms/cm}^3)\) and the plateout surface concentration \(S(\text{atoms/cm}^2)\). The optional sorption characteristics are:
   - Linear sorption with saturation (LS).
   - Freundlich (F) sorption.
   - Langmuir (LA) sorption.
   - Combined Langmuir-Freundlich (LAF) sorption.
The terms in the sorption equations are branch dependent to allow different sorption materials. In addition, the options for "only adsorption" (perfect sink in the plateout surface) and "only desorption" (nothing sticks on the plateout surface) in different branches starting at arbitrary time points may be exercised.

4. Breaking of branch junctions can be modeled. A number of pipe junctions may be broken at chosen time points. Boundary conditions for the free upstream branch ends that result from these failures must be supplied.

5. Input data is kept to a minimum. Only principal parameters such as coolant mass flow rates, temperatures, pressures, hydraulic diameters, etc., are read in. Flow velocities and mass transfer coefficients are computed from these parameters.

6. For the calculation of the mass transfer coefficients time-dependent options for either forced or natural convection are available. The geometry options for forced convection are:

   a. tube flow and annular flow;
   b. aligned tube bundles in cross flow;
   c. non-aligned tube bundles in cross flow;
   d. flat plate;

and for natural convection they are:

   a. tube flow and annular flow;
   b. horizontal tube banks and flat plates;
   c. vertical tube banks and flat plates.
7. Except for the coolant pressure and the coolant and conduit
temperatures, which are restricted to a linear change
along the branch, all other spatially-dependent variables
may change arbitrarily from nodal point to nodal point
within a branch.

6.2 EXPLANATION OF INPUT DATA

This section explains certain details of the input to PADLOC that may
not be obvious in the card image descriptions which follow. In particular,
explanations are given of the following topics.

- Network Geometry
- Boundary Conditions
- Time Points and Time Steps
- Options for Time-Dependent Input
- Spatially-Dependent Input

6.2.1 Network Geometry

6.2.1.1 Configuration

The network is fully characterized by three input parameters. These
are:

NB = number of branches,
NG = number of global nodal points,

and the global point designations for the branch ends,

((IBEIPT(J,IB),J=1,2),IB=1,NB)

The positive x direction, hence the positive flow direction, is defined
as proceeding from the J=1 node toward the J=2 node. The way to determine
these parameters for some typical networks will be shown with several
examples.
Example 1

Consider first the following network of $NB = 7$ branches, designated as (IB). Global points are defined as either branch connection points or free branch end points. These are designated as (IG). In this example the total number of global points is $NG = 7$. The numbering of the global points is arbitrary except that they have to be numbered consecutively from 1 through $NG$. The branch end designations $IBEIPT(J,IB)$ are the upstream ($J=1$) and downstream ($J=2$) global point numbers for the assumed positive flow directions. With these designations, the positive $x$ direction in the branch is established from global point $IG = IBEIPT(1,IB)$ to $IG = IBEIPT(2,IB)$ as shown in the sketch. For sketch 1, the end points are then

Sketch 1. Arrows indicate positive $x$ and flow directions.
Example 2

For the following network

\[ \text{Sketch 2.} \]

\[ \text{NB} = 3 \]
\[ \text{NG} = 4 \]

and

<table>
<thead>
<tr>
<th>IB</th>
<th>IBEIPT(1,IB)</th>
<th>IBEIPT(2,IB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>7</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>4</td>
</tr>
</tbody>
</table>
6.2.1.2 Restrictions

The only restrictions on the networks are

- At $t=0$ there are no free (unconnected) branches permitted unless the network consists of a single branch only.* For example the following initial network geometry is not permitted:

* Later during the run ($t>0$) junctions may be broken and free branches are allowed.
A closed loop has to consist of at least two branches. For example

![Diagram]

is permitted, and

![Diagram]

is not permitted.

6.2.2 Boundary Conditions

6.2.2.1 Regular Network

A boundary condition has to be applied to any global point IG that is a free upstream branch end. The total number of such global points is designated NGBC and the incoming fission product mass flow rate (moles/sec) is BAFRTE(IG). NGBC and BAFRTE are input parameters. For the previously discussed networks of Section 6.2.1.1 these values would be

<table>
<thead>
<tr>
<th>Example</th>
<th>NGBC</th>
<th>IG</th>
<th>BAFRTE(IG)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
<td>&gt; 0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>4</td>
<td>≥ 0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>-</td>
<td>≥ 0</td>
</tr>
</tbody>
</table>

The number of boundary conditions and the incoming fission product mass flow rates may change with time. For example, the coolant flow rates of branches 1, 6, and 7 of sketch 1 (Section 6.2.1.1) might change as shown on the following page.
Of course, if the coolant flows are negative, so are the incoming fission product rates. The appropriate time-dependent boundary conditions are then as described in the table below.

<table>
<thead>
<tr>
<th>IT</th>
<th>NGBC</th>
<th>IG</th>
<th>BAFRTE(IG)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,3</td>
<td>1</td>
<td>2</td>
<td>≥ 0</td>
</tr>
<tr>
<td>4,5</td>
<td>2</td>
<td>1</td>
<td>&lt; 0</td>
</tr>
<tr>
<td>≥ 6</td>
<td>1</td>
<td>1</td>
<td>≤ 0</td>
</tr>
</tbody>
</table>

It is noted that if the value of the boundary condition, BAFRTE, is time dependent, then it must be specified for all time points \( t > 2 \). Further explanation of this is given in Section 6.2.4.

6.2.2.2 Network with Broken Junctions

If branch junctions are to break, additional boundary conditions must be imposed. Breaking of the junction is defined to mean that branches with coolant flows coming into the junction break off. Consider, for example, the following junction IG.
If junction IG breaks, branch 1 breaks off and a boundary condition for branches 2 and 3 must be applied at node IG. If the flows were in the opposite direction, branches 2 and 3 would break off and the imposed boundary condition would apply to branch 1. Once branches are broken at a junction they cannot be connected back again. Also, the imposed boundary fission product flow rate cannot thereafter be changed with time.

The following input into PADLOC is needed to describe junction failures.

1. NDISCT = number of time points IT at which junctions are to break.
2. IT = (ITDISC(J), J=1, NDISCT) are the time points, and,
3. (NDISC(J), J=1, NDISCT) are the number of junctions to break at the time points ITDISC(J).

At each of the time points IT = ITDISC(J), NDISC(J) global point numbers and boundary conditions have to be supplied.

The specification of broken junctions will now be illustrated for the network of Example 1, page 53.

Assume that junction 5 breaks at IT = 2, junction 3 breaks at IT = 5, and junctions 4 and 6 break at IT = 7. Thus,

NDISCT=3, ITDISC(1)=2, \quad NDISC(1)=1
(2)=5, \quad (2)=1
(3)=7, \quad (3)=2.
Assuming that the flow directions are constant in time, the number of boundary conditions and the global points for which they have to be specified are then:

<table>
<thead>
<tr>
<th>IT</th>
<th>NGBC</th>
<th>IG</th>
<th>BAFRTE(IG)</th>
<th>Typical Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>&gt; 0</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>IT</th>
<th>NGBC</th>
<th>IG</th>
<th>BAFRTE(IG)</th>
<th>Broken Junction Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>5</td>
<td>&gt; 0</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>3</td>
<td>&gt; 0</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4, 6</td>
<td>4, 6</td>
<td>&gt; 0, &gt; 0</td>
<td></td>
</tr>
</tbody>
</table>

The boundary conditions for broken junctions are logically separated from the typical boundary conditions because the broken junctions affect the numbers of global points of the network.

6.2.3 Time Points and Time Steps

The time history is divided into NDELT time steps of variable lengths FDELTS as shown on the following page. The time points are designated IT. Time step IT is defined as the interval between time point IT and time point IT + 1.

Many different variables such as mass flows and temperatures can, by option, be specified as functions of time. Most such functions are defined by their numerical values at the NDELT+1 discrete time points, with a piecewise linear variation in the interval tacitly assumed. There are two exceptions to this. First, the length of a time step, FDELTS, refers naturally to an interval, not a point, and only NDELT interval values are specified. Second, boundary conditions are not required at time point 1 (zero time) because here the initial conditions prevail. NDELT boundary conditions are specified for the end of each step, referring to time points 2 through NDELT + 1.
The way in which the program reads the time-dependent input will now be briefly described. At time point 1 the temperatures, flows, and initial concentrations are read in to establish the starting state. Then the program executes a loop over NDELT time steps. The objective during each time step IT is to project the state solution to the next time point, IT + 1. In order to do this using the implicit method, boundary conditions, temperatures, and flows for time point IT + 1 are read in at the start of calculational step IT. The program continues reading ahead in this manner, completing the input for time point NDELT + 1 at the start of step NDELT.

It is noted that the PADLOC solution is influenced by the size of the time step. For the integration parameter θ=0 (explicit solution) the time steps should be chosen in such a way that

\[ \Delta t \lesssim \left( \frac{\Delta x_k}{v_k} \right) \text{min} \]
in any branch (k is the node index). For $0 < \theta < 1$ (implicit solution) one has to avoid a situation where the matrices $B_{22}$ or $D_{22}$ of the partitioned branch systems (p. 36 and 38) become singular. This leads to the following criterion involving $\Delta t$:

$$\theta \Delta t \left[ \left( \frac{p}{\Delta} \right) h_k^l + \left( \frac{|v_k^l|}{\Delta} \right) x_m^l + \left( \frac{\Lambda_c^l}{\Delta} - \theta \Delta t \xi_k^l \right) \right] \neq 1, \; 2 \leq k \leq n-1^*$$

Here,

$$\xi_k^l = \frac{\left( \frac{p}{\Delta} \right) (h^2 \psi)_k^l}{1 + \theta \Delta t (h_k^l \psi_k^l + \lambda)}$$

$$\left( \frac{\Lambda_c^l}{\Delta} \right)_k = \lambda + \left( \frac{\partial v^l}{\partial x} \right)_k + \frac{v_k^l}{A_k^l} \left( \frac{dA}{dx} \right)_k$$

and

$$m = \begin{cases} 
  k-1, & v_k > 0 \\
  k, & v_k < 0 
\end{cases}$$

The above criterion can be satisfied only for certain specific values of the time step $\Delta t$.

PADLOC automatically checks above criteria for $\theta=0$ and $\theta>0$ and, if necessary, recommends an acceptable time step.

6.2.4 Options for Time-Dependent Input

Several options are provided to allow a considerable reduction of input data for certain time-dependent variables. These options are described below.

1. Option for coolant flow rates, coolant pressures, coolant temperatures, and conduit temperatures.

* $l$ is time point index.
(a) ICCWFC=0: All the above variables except the coolant flow rates are assumed to be constant. Coolant flow rates may change from IT=2 on. The number of time points for which new flows are to be read is NFRVSE. The time points of the changes are:

\[ IT = (ITCHF(J), J=1, NFRVSE), ITCHF(J) \geq 2. \]

Consider the following example.

For the above case of a two-branch network,

\[ NFRVSE=3, \quad ITCHF(1)=4 \]
\[ ITCHF(2)=5 \]
\[ ITCHF(3)=8 \]

and the coolant flows of both branches are read for IT=1 and IT=(ITCHF(J), J=1, 3).

(b) ICCWFC=1: All the above variables are read for each time point.
2. Options for Boundary Conditions

ICBC=0: Boundary conditions, if any, are only read for the time point IT=2 and for specified time points IT>2 when they change. In the case of an unbroken network the number of boundary conditions read for each of these time points is NGBC(IT).

An arbitrary number NTGBC of time points IT = ITCHBC(I) > 2 (I=1,NTGBC), at which boundary conditions change, can be specified. If junctions break, additional boundary conditions are required. An arbitrary number NDISCT of time points IT = ITDISC(J) ≥ 2 (J=1,NDISCT), at which junction breaks occur, can be specified. For each of these time points NDISC(J) additional boundary conditions are then read.

ICBC=1: Boundary conditions are read for all time points IT>2.
The total number of boundary conditions for an unbroken network at time point IT is again NGBC(IT). Boundary conditions due to junction breaks are treated the same way as for ICBC=0.

3. Options for Forced and Natural Convection

IGFGN=0: The flags KGF and KGN indicating forced or natural convection and hydrodynamic flow geometry are only read for IT=1 and the convection within a branch is assumed to be either forced or natural throughout a run.

IGFGN=1: The flags are read for all time points IT>1 and the convection patterns may change from time point to time point.

4. Options for Source Rates

IQ12=0: Coolant and plateout source rates are assumed to be independent of time and are only read for IT=1.

IQ12=1: Source rates are read for all time points IT>1.
6.2.5 **Spatially Dependent Input**

The variables

- CPRESS (coolant pressure)
- CTEMP (coolant temperature), and
- WTEMP (conduit wall temperature)

may only change linearly along the branch. The rest of spatially dependent input may change from nodal point to nodal point. For constant values along x, only the value at x=0 (J=1 end of the branch) need be read in most cases. For linearly changing variables the values at x=0 and x=L are read. In particular, the following options are provided to facilitate this input:

1. **Option for Δx (Mesh Spacing) Values**
   
   IX=0: All Δx values of the branch are assumed to be of equal length. Δx is not read but is computed from the branch length and the number of nodes.

   IX=1: (NODES-1) Δx values are read for the branch. NODES is the total number of nodes on the branch, including end points.

2. **Options for Hydraulic Diameters and Conduit Cross Sections**
   
   a. KCIR=0: Assumes circular cross section with linearly changing hydraulic diameter DHD.

      For constant DHD, only DHD(x=0) need be read. Otherwise, the hydraulic diameters at both branch ends must be read.

   b. KCIR=1: Assumes arbitrary cross section (including circular). Both the hydraulic diameters and cross sectional areas need to be read.

If NHD=0, these values are assumed constant along the branch and are only read for x=0. For NHD=1 they are read for each nodal point.
3. **Options for Initial Concentrations**

INIT(1,IB) and INIT(2,IB) are options for the coolant and plateout concentrations, respectively.

- **INIT(1,IB)=0:** The initial coolant concentrations of branch IB are assumed to be zero and are not read.

- **INIT(1,IB)=1:** The initial coolant concentration is constant along the branch, and its value at the first nodal point is read.

- **INIT(1,IB)=2:** The initial coolant concentration changes linearly along the branch. The concentrations at the first and last nodal points are read.

- **INIT(1,IB)=3:** The initial coolant concentration changes arbitrarily along the branch, and the values at all nodal points are read.

INIT(2,IB)= is the corresponding flag for the initial plateout concentration of branch IB.

4. **Source Rate Options**

- **JQ1=0:** The coolant source rate of branch IB is zero and is not read.

- **JQ1=1:** The coolant source rate is constant along the branch, and only the value at the first node is read.

- **JQ1=2:** The coolant source rate changes linearly along the branch, and its values at the first and last branch nodes are read.
JQ1=3: The coolant source rate changes arbitrarily along the branch and, its values at all nodal points are read.

\[
\begin{cases}
0 \\
1 \\
2 \\
3
\end{cases}
\]

is the corresponding flag for the plateout source rate.

6.2.6 Sorption Equations

In the following equations the units for the boundary layer concentrations, surface concentrations, and vapor pressures are

\[
[B] = \text{atoms/cm}^3 \\
[S] = \text{atoms/cm}^2 \\
[p] = \text{atm}
\]

1. Linear Sorption with Saturation (LS)

According to the ideal gas law,

\[
B_{LS} = \frac{N_A}{RT} p(T), \quad (64)
\]

where

- \(N_A\) is Avogadro's number (atoms/g-mole)
- \(R\) is the gas constant (cm\(^3\) atm/(g-mole \(^0\)K))
- \(T\) is the temperature (\(^0\)K)

the vapor pressure \(p(T)\) adjacent to the conduit surface is given by

\[
p(T) = \frac{S}{S_s} 10^{AVPOR - \frac{BVPOR}{T_w}} \quad (S < S_s)
\]

or

\[
p(T) = 10^{AVPOR - \frac{BVPOR}{T_w}} \quad (S \geq S_s)
\]
where $S$ is the surface concentration, and $S_s$ is a saturation surface concentration.

2. **Freundlich (F) Sorption**

$$B_F = \frac{N_A}{RT} \rho(T),$$

where

$$\rho(T) = e^{F(T)} = e^{ACP} + \frac{BCP}{T}, \quad \text{and}$$

$$\gamma_F(T) = CCP + \frac{DCP}{T}.$$ (66)

3. **Langmuir (LA) Sorption**

$$B_{\text{LA}} = \frac{N_A}{RT} \rho(T),$$

where

$$\rho(T) = \beta_{\text{LA}}(T) S,$$ (67)

$$\beta_{\text{LA}}(T) = \beta_F(T) S_t^{\gamma_F(T)-1}, \quad \text{and}$$

$S_t$ is the plateout transition concentration between the Langmuir and Freundlich regimes.
4. **Combined Langmuir-Freundlich (LAF) Sorption**

\[ B_{\text{LAF}} = B_{\text{LA}} + B_{\text{F}} \]

where \( B_{\text{LA}} \) and \( B_{\text{F}} \) are defined above in parts 3 and 2, respectively.

Each branch can have one of these four sorption characteristics. Starting with specified time points, dependent on the branch, the sorption behavior can be switched to adsorption only or desorption only. A switch back to normal sorption behavior is not possible.

The case of "adsorption only" is characterized by \( C \gg B \), where \( C \) is the coolant concentration and \( B \) is the boundary layer concentration, respectively. The difference of these concentrations appears in the mass transfer term (flux across the boundary layer)

\[
\text{flux} = h(x,t) [B(x,t) - C(x,t)] \text{, atoms cm}^{-2}\text{ sec}^{-1}
\]

of Eq.(5) and (6) on page 17. Consequently, PADLOC treats "adsorption only" by setting

\[
\text{flux} = -h(x,t) C(x,t)
\]

"Desorption only" is characterized by zero residence time of the fission products on the plateout surface. Thus, PADLOC transfers the contents of the plateout surface to the coolant (as a coolant source rate). In addition, all plateout sources are transferred to the coolant and the plateout concentration is set to zero.

6.3 **INPUT INSTRUCTIONS**

This section contains abbreviated card image input instructions. In cases where more detailed information is required for their understanding, references are made to appropriate discussions and formulae in the preceding section (6.2).
The card data are subdivided into two parts, A and B. Part A (cards A1 to A16) is for time-independent input and describes mainly the branch geometry and the physical sorption properties. Part B (cards B1 to B12) is for time-dependent input such as time steps, coolant mass flow rates, pressures, temperatures, source rates, boundary conditions, etc.

The deck setup necessary to run PADLOC on the UNIVAC-1110 is given below.

Deck Setup

Run Card
ASG,AX PADLOC*2. /Control
XQT PADLOC*2.PADLOC /Cards
Card A1
::
A16
B1
::
B12

Input Cards

The remaining input instructions are given on the following pages.
<table>
<thead>
<tr>
<th>Word</th>
<th>1-6</th>
<th>7-12</th>
<th>13-18</th>
<th>19-24</th>
<th>25-30</th>
<th>31-36</th>
<th>37-42</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
</tr>
<tr>
<td>Format</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
<td>I6</td>
</tr>
<tr>
<td>Card</td>
<td>Number of branches that make up the global pipe network.</td>
<td>Number of global nodal points of the network.</td>
<td>The maximum number of branches meeting at any global nodal point.</td>
<td>Number of time points IT&gt;2 for which new boundary conditions are to be read if ICBC=0 (NTGBC≥0). See A5 for ICBC and Section 6.2.4.</td>
<td>The maximum number of nodes (including end nodes) in any branch</td>
<td>The number of time points for which junction breaks occur (NDISCT&gt;0).</td>
<td>Number of time points for which coolant flow rates are read if ICCWFC=0 (NFRVSE≥0). See A5 for ICCWFC and Section 6.2.4.</td>
</tr>
<tr>
<td>Symbol</td>
<td>NB</td>
<td>NG</td>
<td>NBGP</td>
<td>NTGBC</td>
<td>NDMX</td>
<td>NDISCT</td>
<td>NFRVSE</td>
</tr>
</tbody>
</table>

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<table>
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<tr>
<th>Word</th>
<th>1-6</th>
<th>7-12</th>
<th>etc.</th>
<th>etc.</th>
<th>etc.</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
</tr>
<tr>
<td>Format</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
<td>A6</td>
</tr>
<tr>
<td>Card</td>
<td>Alphanumeric job title. 72 characters maximum</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>TITLE(1)</td>
<td>TITLE(2)</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>TITLE(12)</td>
</tr>
<tr>
<td>Card A3</td>
<td>Symbol</td>
<td>Word</td>
<td>Column</td>
<td>Format</td>
<td>Column</td>
<td>Format</td>
</tr>
<tr>
<td>--------</td>
<td>--------</td>
<td>------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td></td>
<td>NDELT</td>
<td>Number of time steps required for the run.</td>
<td>1-12</td>
<td>I12</td>
<td>13-24</td>
<td>E12.0</td>
</tr>
<tr>
<td></td>
<td>NEDIT</td>
<td>Print results every NEDIT time steps (NEDIT&gt;0).</td>
<td>25-36</td>
<td>E12.0</td>
<td>37-48</td>
<td>E12.0</td>
</tr>
<tr>
<td></td>
<td>THETA</td>
<td>Time integration parameter (0&lt;THETA&lt;1) THETA = 0.0, Fully explicit 1.0, Fully implicit 0.5, Crank Nicholson</td>
<td>3</td>
<td>E12.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ERRS</td>
<td>Relative error for convergence of plate-out concentration. Provide only if at least one of the branches has nonlinear sorption behavior. A recommended value is 10^-6.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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<th>Column</th>
<th>Format</th>
<th>Column</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>XNAME</td>
<td>Alphanumeric nuclide name e.g., Cs-137. Used for print out heading. (Start in Column 1).</td>
<td>1-6</td>
<td>A6</td>
<td>13-24</td>
<td>E12.0</td>
</tr>
<tr>
<td></td>
<td>XLAM</td>
<td>Decay constant (s^-1) (XLAM&gt;0)</td>
<td>25-36</td>
<td>E12.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>WMIS</td>
<td>Molecular mass of isotope e.g., 137.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
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### Card A5

<table>
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<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
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<tbody>
<tr>
<td>Column</td>
<td>1-3</td>
<td>4-6</td>
<td>7-9</td>
<td>10-12</td>
<td>13-15</td>
<td>16-18</td>
</tr>
<tr>
<td>Format</td>
<td>I3</td>
<td>I3</td>
<td>I3</td>
<td>I3</td>
<td>I3</td>
<td>I3</td>
</tr>
</tbody>
</table>

- **Card A5**
  - `=0`, boundary conditions are to change at a few specified time points. `=1`, they are read for all time points \(IT\geq 2\).
  - `=0`, coolant and wall conditions are independent of time. `=1`, otherwise.*
  - `=0`, convection (forced or natural) pattern and hydrodynamic flow geometries are independent of time. `=1`, otherwise.*
  - `=0`, coolant and surface source rates are independent of time. `=1`, otherwise.*
  - Total number of branches that change their sorption behavior during a run to "adsorption only" or "desorption only" \(0 < \text{NADDS} \leq \text{NB}\)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>ICBC</th>
<th>IDELTD</th>
<th>ICCWFC</th>
<th>IC_FGN</th>
<th>IQ12</th>
<th>NADDS</th>
</tr>
</thead>
</table>

* See also Section 6.2.4.

### Information on branches that change their sorption behavior.

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>etc.</th>
<th>etc.</th>
<th>etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-6</td>
<td>7-12</td>
<td>13-24</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
</tr>
<tr>
<td>Format</td>
<td>I6</td>
<td>I6</td>
<td>I12</td>
<td>I6</td>
<td>I6</td>
<td>I12</td>
</tr>
</tbody>
</table>

- **Card A6**
  - Index of first branch.
  - `= -1`, adsorption only.
  - `= 1`, desorption only.
  - Time point \(IT\) at which the new sorption behavior starts.
  - Repeat same information for all branches up to the last branch of index \(IB^\text{NADDS}\).

<table>
<thead>
<tr>
<th>Symbol</th>
<th>IB&lt;sub&gt;1&lt;/sub&gt;</th>
<th>IAD(IB&lt;sub&gt;1&lt;/sub&gt;)</th>
<th>NTSAD(IB&lt;sub&gt;1&lt;/sub&gt;)</th>
<th>IB&lt;sub&gt;NADDS&lt;/sub&gt;</th>
<th>IAD(IB&lt;sub&gt;NADDS&lt;/sub&gt;)</th>
<th>NTSAD(IB&lt;sub&gt;NADDS&lt;/sub&gt;)</th>
</tr>
</thead>
</table>

**Comments**
- Skip A6 if NADDS=0 (A5).
- NTSAD\(>1\) if the initial plateout concentration of the branch is zero. Otherwise NTSAD\(>2\).
- Use as many 6-word cards as required.
### Time points for new coolant flow rates.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Card</th>
<th>Symbol</th>
<th>1-12</th>
<th>13-24</th>
<th>etc.</th>
<th>etc.</th>
<th>etc.</th>
<th>112</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1-12</td>
<td>112</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **A7**: First time point at which coolant mass flow rates change.
- **ITCHF(l)**: See also Section 6.2.4.

### Time points for new boundary conditions.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Card</th>
<th>Symbol</th>
<th>1-12</th>
<th>13-24</th>
<th>etc.</th>
<th>etc.</th>
<th>etc.</th>
<th>112</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1-12</td>
<td>112</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **A8**: First time point at which new boundary conditions apply.
- **ITCHBC(1)**: See also Section 6.2.4.
Time points ITDISC and number of branch connections NDISC that break at these time points.

<table>
<thead>
<tr>
<th>Column</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-12</td>
<td>112</td>
</tr>
<tr>
<td>13-24</td>
<td>etc.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>ITDISC(1)</th>
<th>NDISC(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>A9</td>
<td></td>
</tr>
<tr>
<td>A9</td>
<td>First time point at which branch junctions break.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total number of global points that break at ITDISC(1).</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Last time point at which branch junctions break.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total number of global points that break at ITDISC(NDISC).</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>ITDISC(NDISC)</th>
<th>NDISC(NDISC)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Skip A9 if NDISC=0, A1.</td>
</tr>
</tbody>
</table>

Branch end global point designations.

<table>
<thead>
<tr>
<th>Column</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-3</td>
<td>13</td>
</tr>
<tr>
<td>4-6</td>
<td>etc.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>IBEIPT(1,1)</th>
<th>IBEIPT(2,1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>A10</td>
<td></td>
</tr>
<tr>
<td>A10</td>
<td>Branch 1: Global point number for X=0 end of branch.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Branch 1: Global point number for X=L end of branch.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Branch NB: Global point number at X=0 end of branch.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Branch NB: Global point number at X=L end of branch.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Note: positive flow velocity is defined such that X=0 is upstream and X=L is downstream.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>IBEIPT(1,NB)</th>
<th>IBEIPT(2,NB)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>See A1 for NB. Use as many 6-word cards as required.</td>
</tr>
</tbody>
</table>
Branch Loop: Repeat the set (All to A16) for each branch. Start with branch IB=1 and proceed to IB=NB.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>All</td>
<td>Alphanumeric branch identification 72 characters maximum.</td>
<td>BRNCHN(1,IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>BRNCHN(2,IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>BRNCHN(12,IB)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>A12</td>
<td>Branch length (cm)</td>
<td>BLENCT(IB)</td>
</tr>
<tr>
<td></td>
<td>1-12</td>
<td>E12.0</td>
<td>ENTL(IB)</td>
</tr>
<tr>
<td></td>
<td>13-24</td>
<td>E12.0</td>
<td>NNODES(IB)</td>
</tr>
<tr>
<td></td>
<td>25-27</td>
<td>E12.0</td>
<td>INIT(1,IB)</td>
</tr>
<tr>
<td></td>
<td>28-30</td>
<td>E12.0</td>
<td>INIT(2,IB)</td>
</tr>
<tr>
<td></td>
<td>31-33</td>
<td>E12.0</td>
<td>IX</td>
</tr>
<tr>
<td></td>
<td>34-36</td>
<td>E12.0</td>
<td>KCIR(IB)</td>
</tr>
<tr>
<td></td>
<td>37-39</td>
<td>E12.0</td>
<td></td>
</tr>
</tbody>
</table>

- Branch length (cm)
  - 1. ENTL=hydrodynamic entry length (cm) if KGFP=3 or KGNTT=0. (See B8 and Appendix A for KGFP and KGNTT).
  - 2. ENTL=BLENCT otherwise.
- Number of nodes (including end nodes) for branch. NNODES(IB)≥3.
- =0, if initial coolant concentration C is zero.
- =1, if C=constant along branch.
- =2, if C changes linearly along branch.
- =3, if C arbitrary function along branch.
- =0, if initial plateout concentration S is zero.
- =1, if S=constant along branch.
- =2, if S changes linearly along branch.
- =3, if S arbitrary function along branch.
- =0, if all Δx within branch are of same length.
- =1, otherwise.
- =1 for arbitrary cross section (including circular).
- =0 for circular cross section whose hydraulic diameter changes linearly along branch.
### Constants of the sorption equations (see also Section 6.2.6).

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Column</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>A12</td>
<td>E12.0</td>
<td>1-12</td>
<td>AVPOR(IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13-24</td>
<td>BVPOR(IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>25-36</td>
<td>ACP(IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>37-48</td>
<td>BCP(IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>49-60</td>
<td>CCP(IB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>61-72</td>
<td>DCP(IB)</td>
</tr>
</tbody>
</table>

The constants are provided for different branches IB and include AVPOR, BVPOR, ACP, BCP, CCP, and DCP. The format E12.0 is used for these constants. The variables are defined as follows:

- AVPOR in Eq. (65) for branch IB (LS only).
- BVPOR in Eq. (65) for branch IB (LS only).
- ACP in Eq. (66) for branch IB (F or LA).
- BCP in Eq. (66) for branch IB (F or LA).
- CCP in Eq. (66) for branch IB (F or LA).
- DCP in Eq. (66) for branch IB (F or LA).
### Spatial discretization of branch IB.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Symbol</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>1-12</td>
<td>E12.0</td>
<td>DELX(1,IB)</td>
<td></td>
</tr>
<tr>
<td>A14</td>
<td>13-24</td>
<td>E12.0</td>
<td>DELX(2,IB)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>DELX(N1,IB)</td>
<td></td>
</tr>
</tbody>
</table>

- DELX = Δx(cm) at the upstream end of branch.
- DELX(N1,IB) = Δx(cm) at the downstream end of branch.
- N1 = number of nodes minus 1.
- Use as many 6-word cards as required.
- Skip A14 if IX=0, A12.

### Card A13 Cont'd

- Constant $S_t$ in Eq. (67) for Langmuir sorption behavior.
- If LANGMR=1 and LFREUN=1, STRAN is the transition plateout concentration from Langmuir to Freundlich regime.
- 1-12 E12.0

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Symbol</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>1-12</td>
<td>E12.0</td>
<td>STRAN(IB)</td>
<td></td>
</tr>
<tr>
<td>A13</td>
<td>13-24</td>
<td>E12.0</td>
<td>SSAT(IB)</td>
<td></td>
</tr>
</tbody>
</table>

- Constant $S_s$ in Eq. (64) for linear sorption with saturation.
- $S_s$ is the saturation concentration of the plateout surface of branch IB.
- 1-12 E12.0

- Provide only those constants needed for the chosen sorption equation.
- Use two 6-word cards.

### Comments

- Provide only those constants needed for the chosen sorption equation.
- Use two 6-word cards.
Circular pipe with linear change of diameter DHD.

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
<th>2</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-12</td>
<td>13-24</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Skip A15 if KCIR(IB)=1, A12.</td>
</tr>
<tr>
<td>Format</td>
<td>E12.0</td>
<td>E12.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card A15</td>
<td>Inner pipe diameter (cm) at upstream end of branch.</td>
<td>Inner pipe diameter (cm) at downstream end of branch. Leave blank for constant DHD along branch.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>DHD(1,IB)</td>
<td>DHD(2,IB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Arbitrary conduit (including circular)

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
<th>2</th>
<th>etc.</th>
<th>2*N-1</th>
<th>2*N</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-12</td>
<td>13-24</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>Skip A16 if KCIR(IB)=0, A12.</td>
</tr>
<tr>
<td>Format</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td>E12.0</td>
<td></td>
</tr>
<tr>
<td>Card A16</td>
<td>Hydraulic diameter (cm) at upstream end of branch. (See Appendix A for definition).</td>
<td>Cross section area (cm^2) at upstream end of branch.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>DHD(1,IB)</td>
<td>CROSSA(1,IB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>DHD(2,IB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>DHD(N,IB)</td>
<td>CROSSA(N,IB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
To summarize the logic for reading the time-dependent input parameters on cards B1 to B12, the diagram below is provided for guidance. The diagram shows the loop over the time points IT and the branch loop over branches IB. The time points and flags for which the cards are to be provided are also specified.

```
    DO 100 IT=1,NDELT+1 (time point loop)
        B1  read for \{ IT=1
           \quad \{ 2<IT<NDELT if IDELTD=1
                   \quad \{ IT=1
                        \quad \{ 2<IT<NDELT+1 if ICCWFC=1, or
                                   \quad \quad IT(J)=ITCHF(J)>2 if ICCWFC=0
                                   \quad \quad IT=2 and IT=ITCHBC>2 if ICBC=0
                                   \quad \} IT=1,IT=ITCH(J)>2
                        \} IT=1,IT=ITCH(J)>2
        B2  read for \{ IT=1
           \quad \{ 2<IT<NDELT+1 if ICCWFC=1, or
                   \quad \quad IT(J)=ITCHF(J)>2 if ICCWFC=0
                   \quad \} IT=1,IT=ITCH(J)>2
        B3  read for \{ time points IT for which B3 was read
           \quad \} provided NGBC>1
        B4  read for \{ IT(J)=ITDISC(J)>2
           \quad \} provided NDISCT>1
        B5  read for \{ IT=1
           \quad \{ 2<IT<NDELT+1 if IGFGN=1
                   \} IT=1
        B6  read for IT=1 if INIT(1,IB)=1
        B7  read for IT=1 if INIT(2,IB)=1
        B8  read for IT=1
           \quad \{ 2<IT<NDELT+1 if IGFGN=1
                   \} IT=1
        B9  read for \{ IT=1
           \quad \{ 2<IT<NDELT+1 if ICCWFC=1
                   \} IT=1
        B10 read for \{ IT=1
           \quad \{ 2<IT<NDELT+1 if IQ12=1
                   \} IT=1
        B11 read if B10 was read and JQ1>1
        B12 read if B10 was read and JQ2>1
    CONTINUE
```
### Card B1

**Time step [s] between time points IT and IT+1.**

Symbol: FDELT

### Coolant mass flow rates [g/s] for branches IB=1 to IB=NB.

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
<th>2</th>
<th>etc.</th>
<th>NB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-12</td>
<td>13-24</td>
<td>etc.</td>
<td>etc.</td>
</tr>
<tr>
<td>Format</td>
<td>E12.0</td>
<td>E12.0</td>
<td>etc.</td>
<td>etc.</td>
</tr>
</tbody>
</table>

#### Card B2

**Coolant mass flow rate [g/sec] for branch 1.**

**Positive flow is in positive X direction, from 0 to L.**

Symbol: FLORTE(1) FLORTE(2) etc. FLORTE(NB)
Number of boundary conditions at time point IT. NGBC does not include additional boundary conditions required due to breaking of branch junctions.

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-3</td>
</tr>
<tr>
<td>Format</td>
<td>I3</td>
</tr>
<tr>
<td>Card B3</td>
<td>Total number of boundary conditions required for the unbroken network at time point IT. NGBC&gt;0</td>
</tr>
</tbody>
</table>

Symbol: NGBC

Comments:

Provide B3 for
1) \(2 < IT < NDELT+1, ICBC=1\).
2) \(IT=2\) and \(IT(J)=IUCHBC(J)>2, ICBC=0\).
See also loop diagram on page 79 and Sections 6.2.2 and 6.2.4.

Global point numbers IG and corresponding boundary fission product flow rates \(BAFRTE(IG)\) [moles/s] for boundary conditions required at time point IT. Boundary conditions due to breaking of branch connections are not included.

<table>
<thead>
<tr>
<th>Word</th>
<th>1</th>
<th>2</th>
<th>etc.</th>
<th>2*NGBC-1</th>
<th>2*NGBC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>1-12</td>
<td>13-24</td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
</tr>
<tr>
<td>Format</td>
<td>I12</td>
<td>E12.0</td>
<td>etc.</td>
<td>I12</td>
<td>E12.0</td>
</tr>
<tr>
<td>Card B4</td>
<td>Global nodal point number for which boundary condition is applied. See also Section 6.2.2.</td>
<td>Fission product mass flow rate coming into global point IG. See also Section 6.2.2.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symbol: IG

Comments:

Provide B4 if B3 is read and NGBC>0. See also loop diagram on page 79. Use as many 6-word cards as required.
Loop over branch connections that break at time point IT. Provide NDISC(J) cards B5 at each of the time points.

IT = ITDISC(J). See A9 for NDISC and ITDISC.

<table>
<thead>
<tr>
<th>Card</th>
<th>Global point that breaks at IT = ITDISC(J).</th>
</tr>
</thead>
<tbody>
<tr>
<td>B5</td>
<td>New fission product flow rate (moles/sec) at IG for all branches IB whose upstream end global point is IG.</td>
</tr>
</tbody>
</table>

Symbol: IG, BAFRTE(IB)

B6 to B12 are within the branch loop. Start with IB = 1 and proceed to IB = NB.

Initial conditions read only at first time point.

<table>
<thead>
<tr>
<th>Card</th>
<th>Initial coolant concentration (atoms/cm(^3)) at the upstream node of branch IB at zero time.</th>
</tr>
</thead>
<tbody>
<tr>
<td>B6</td>
<td>etc.</td>
</tr>
</tbody>
</table>

Symbol: C(1,IB), C(2,IB), ..., C(N,IB)

Comments
- Provide B5 for IT = ITDISC(J) > 2 if NDISCT > 0.
- Skip B5 if NDISCT = 0 (A1).
- See also loop diagram on page 79 and Section 6.2.2.2.

Comments
- Provide B6 only if at least one node has a non-zero concentration (INIT(1,IB) > 0)
- N = 1 if C is constant along branch
- N = 2 for linear change of C along branch
- N = NNODES(IB) for C = arbitrary function along branch
- Use as many 6-word cards as required.
Initial conditions read only at first time point.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>1-2</th>
<th>13-24</th>
<th>etc.</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>B7</td>
<td>1-12</td>
<td>E12.0</td>
<td></td>
<td></td>
<td>etc.</td>
<td>etc.</td>
</tr>
<tr>
<td></td>
<td>13-24</td>
<td>E12.0</td>
<td></td>
<td></td>
<td>etc.</td>
<td>etc.</td>
</tr>
</tbody>
</table>

Card B7

Initial plate-out concentration (atoms/cm²) at the upstream node of branch IB at zero time.

Initial plate-out concentration (atoms/cm²) at the downstream node of branch IB at zero time.

Symbol

| S(1,IB) | S(2,IB) | etc. | S(N,IB) |

Flow condition flags.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>1-3</th>
<th>4-6</th>
<th>7-9</th>
</tr>
</thead>
<tbody>
<tr>
<td>B8</td>
<td>1-3</td>
<td>I3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4-6</td>
<td>I3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7-9</td>
<td>I3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Card B8

=0, natural convection. 0, forced convection. 0, forced convection.

1<KGF<4, forced convection. 1<KGN<3, natural convection. 1, if KGN>2 and flat plate

Symbol

| KGF(IB) | KGN(IB) | KGNFP(IB) |

Comments

Provide B7 only if at least one node has a non-zero concentration (INIT(2,IB)>0). N=1 if S is constant along branch. N=2 if S changes linearly along branch. N=NNODES(IB) for S = arbitrary function along branch.

Use as many 6-word cards as required.

Comments

Provide B8 for

1) IT=1.
2) 2<IT<NDELT+1 if IGFGN=1.

See also loop diagram on page 79 and tables 1 and 2 of Appendix A.
Linearly changing pressures and temperatures.

<table>
<thead>
<tr>
<th>Word</th>
<th>Column</th>
<th>Format</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card</td>
<td>B9</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Coolant pressure [atm] at (x=0).</td>
<td>E12.0</td>
<td>CPRESS(1,IB)</td>
</tr>
<tr>
<td></td>
<td>Leave blank if pressure constant along branch.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Coolant pressure [atm] at (x=L).</td>
<td>E12.0</td>
<td>CPRESS(2,IB)</td>
</tr>
<tr>
<td></td>
<td>Coolant temperature [°C] at (x=0).</td>
<td>E12.0</td>
<td>CTEMP(1,IB)</td>
</tr>
<tr>
<td></td>
<td>Leave blank if coolant temperature constant along branch</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Coolant temperature [°C] at (x=L).</td>
<td>E12.0</td>
<td>CTEMP(2,IB)</td>
</tr>
<tr>
<td></td>
<td>Leave blank if wall temperature constant along branch</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Wall temperature [°C] at (x=0).</td>
<td>E12.0</td>
<td>WTEMP(1,IB)</td>
</tr>
<tr>
<td></td>
<td>Leave blank if wall temperature should be same as coolant temperature.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Wall temperature [°C] at (x=L).</td>
<td>E12.0</td>
<td>WTEMP(2,IB)</td>
</tr>
</tbody>
</table>

Comments

Provide B9 for
1) \(I=1\).
2) \(2<IT<NDEL+1\) if ICCWFC=1.
See also loop diagram on page 79.
\(L=\) branch length.
## Source rate flags.

<table>
<thead>
<tr>
<th>Word</th>
<th>1-3</th>
<th>4-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>=0, no coolant source.</td>
<td>=0, no coolant source.</td>
</tr>
<tr>
<td>Format</td>
<td>=1, coolant source rate is constant along branch.</td>
<td>=1, coolant source rate is constant along branch.</td>
</tr>
<tr>
<td>Card B10</td>
<td>=2, source rate changes linearly along branch.</td>
<td>=2, source rate changes linearly along branch.</td>
</tr>
<tr>
<td>Symbol</td>
<td>JQ1</td>
<td>JQ2</td>
</tr>
</tbody>
</table>

### Comments
Provide B10 for IT=1, and, if IQ12=1, also for 2<IT<NDELT +1. See A5 for IQ12.

<table>
<thead>
<tr>
<th>Word</th>
<th>1-12</th>
<th>13-24</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column</td>
<td>=0, no plateout source rate.</td>
<td>=0, no plateout source rate.</td>
</tr>
<tr>
<td>Format</td>
<td>=1, source rate is constant along branch.</td>
<td>=1, source rate is constant along branch.</td>
</tr>
<tr>
<td>Card B11</td>
<td>=2, source rate changes linearly along branch.</td>
<td>=2, source rate changes linearly along branch.</td>
</tr>
<tr>
<td>Symbol</td>
<td>Q(1,1,IB)</td>
<td>Q(2,1,IB)</td>
</tr>
</tbody>
</table>

### Comments
Provide B11 only if at least one node has non-zero source rate (JQ1>1).

- N=1 if Q is constant along branch
- N=2 if Q changes linearly along branch
- N=NNODES(IB) for Q being arbitrary function along branch.

Use as many 6-word cards as required.
<table>
<thead>
<tr>
<th>Word</th>
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<td>E12.0</td>
<td>Plateout source rate (atoms/(cm²sec)) at branch end x=0.</td>
</tr>
<tr>
<td></td>
<td>13-24</td>
<td>E12.0</td>
<td>etc.</td>
</tr>
<tr>
<td></td>
<td>etc.</td>
<td>etc.</td>
<td>etc.</td>
</tr>
<tr>
<td>N</td>
<td>etc.</td>
<td>etc.</td>
<td>Plateout source rate (atoms/(cm²sec)) at branch end x=L.</td>
</tr>
</tbody>
</table>

| Symbol | Q(1,2,IB) | Q(2,2,IB) | Q(N,2,IB) |

Comments
Provide B12 only if at least one node has non-zero source (JQ2≥1). N=1 if Q is constant along branch. N=2 if Q changes linearly along branch. N=NNODES(IB) if Q is arbitrary function along branch.

Use as many 6-word cards as required.
7. SAMPLE PROBLEMS

7.1 INTRODUCTION

In this section we shall present a few sample problems. The intention is to demonstrate the PADLOC capabilities and to verify the code by comparison with analytical solutions. For this purpose we shall derive some exact solutions in Section 7.2. For convenience, two simplified cases will be considered. The first will deal with pure time dependence by assuming all parameters around a closed circuit are independent of position. The second will deal with pure space dependence via a steady-state solution. The comparison of PADLOC results with the exact solutions will then be presented in Section 7.3.

7.2 ANALYTICAL SOLUTIONS

For simplicity we assume that the source rates and all flow parameters are independent of space and time. This implies that the pipe geometry is also independent of the axial distance $x$. The equations (5) and (6) for the coolant and plateout concentrations are then

$$
\frac{\partial C(x,t)}{\partial t} = q_c + \frac{P}{A} h \left[ B(x,t) - C(x,t) \right] - v \frac{\partial C(x,t)}{\partial x} - \lambda C(x,t) , \quad (69)
$$

$$
\frac{\partial S(x,t)}{\partial t} = q_s - h \left[ B(x,t) - C(x,t) \right] - \lambda S(x,t) . \quad (70)
$$

7.2.1 Time Dependence Only

To check the time dependence of PADLOC results we will first derive a solution that depends only on time. A practical example is a closed loop with uniform parameters. It is clear that the concentrations of a decaying nuclide in such a loop will be independent of the spatial distance $x$. This means that $\partial C/\partial x = 0$ in Eq. (69), and the equations simplify to
\[
\frac{dC(t)}{dt} = q_c + \frac{P}{A} h \left[ B(t) - C(t) \right] - \lambda C(t) , \quad (71)
\]

\[
\frac{dS(t)}{dt} = q_s - h \left[ B(t) - C(t) \right] - \lambda S(t) . \quad (72)
\]

Multiplying Eq. (72) by \( P/A \) and adding the result to Eq. (71), one obtains

\[
\frac{d}{dt} \left[ C(t) + \frac{P}{A} S(t) \right] = \left[ q_c + \frac{P}{A} q_s \right] - \lambda \left[ C(t) + \frac{P}{A} S(t) \right] . \quad (73)
\]

This suggests a change of variable for further simplification. Defining

\[
U(t) \equiv C(t) + \frac{P}{A} S(t) , \quad \text{and} \quad (74)
\]

\[
\dot{Q}_1 \equiv \dot{q}_c + \frac{P}{A} \dot{q}_s , \quad (75)
\]

Eq. (73) becomes

\[
\frac{d}{dt} U(t) + \lambda U(t) = \dot{Q}_1 . \quad (76)
\]

The solution to Eq. (76) is

\[
U(t) = U(o) e^{-\lambda t} + \frac{\dot{Q}_1}{\lambda} \left( 1 - e^{-\lambda t} \right) , \quad (77)
\]

where

\[
U(o) = C(o) + \frac{P}{A} S(o) . \quad (78)
\]

We shall return to the intermediate solution \( U(t) \) later.

Let us now make an additional simplification to eliminate \( B(t) \) from Eq. (71). Assuming linear sorption behavior,

\[
B(t) = \alpha + \beta S(t) . \quad (79)
\]
Substituting (79) into (71) then gives

$$\frac{dC(t)}{dt} = q_c \frac{P}{A} h \left[ \alpha + \beta S(t) - C(t) \right] - \lambda C(t) .$$ \hspace{1cm} (80)

We can eliminate S(t) in favor of U(t), a known function of time, by substituting Eq. (74) into Eq. (80). Doing this and collecting terms, the result is

$$\frac{dC(t)}{dt} = \dot{Q}_2 - \omega C(t) + h \beta U(t) ,$$ \hspace{1cm} (81)

$$\omega \equiv h \left( \beta + \frac{P}{A} \right) + \lambda , \hspace{1cm} \text{and} \hspace{1cm}$$ \hspace{1cm} (82)

$$\dot{Q}_2 \equiv \dot{q}_c + \frac{P}{A} h \alpha .$$ \hspace{1cm} (83)

We can now eliminate the known U(t) from Eq. (81) to obtain a differential equation in C(t) alone. Substituting (77) and (78) into (81), we finally obtain

$$\frac{dC(t)}{dt} + \omega C(t) = A + B e^{-\lambda t} ,$$ \hspace{1cm} (84)

where

$$A \equiv \dot{Q}_2 + \frac{h \beta \dot{Q}_1}{\lambda}$$ \hspace{1cm} (85)

and

$$B \equiv h \beta \left[ C(o) + \frac{P}{A} S(o) - \frac{\dot{Q}_1}{\lambda} \right]$$ \hspace{1cm} (86)

are both known from the given source rates and initial conditions. The solution to (84) is

$$C(t) = C(0) e^{-\omega t} + \frac{A}{\omega} \left( 1 - e^{-\omega t} \right) + \frac{B}{\omega - \lambda} \left( e^{-\lambda t} - e^{-\omega t} \right) .$$ \hspace{1cm} (87)
This completes the solution. As it stands Eq. (87) is not defined for \( \omega=\lambda \) (\( h=0 \)) or \( \omega=0 \) (\( h=0 \) and \( \lambda=0 \)). These special cases are easily treated by applying l'Hopital's rule to find the appropriate limits, but the details need not be given here.

7.2.2 Spatial Dependence Only

The spatial dependence can be obtained by solving the system (69), (70) for steady-state conditions. In this case \( \partial C/\partial t = \partial S/\partial t = 0 \) and the equation system reduces to

\[
\begin{align*}
q_c + \frac{h}{A} \left[ B(x) - C(x) \right] - v \frac{dC(x)}{dx} - \lambda C(x) &= 0, \quad (88) \\
\frac{dS(x)}{dx} - h \left[ B(x) - C(x) \right] - \lambda S(x) &= 0. \quad (89)
\end{align*}
\]

First consider a stable isotope (\( \lambda=0 \)):

From (89) we obtain

\[
h \left[ B(x) - C(x) \right] = \dot{q}_s. \quad (90)
\]

Substituting (90) into (88) yields

\[
\frac{dC(x)}{dx} = \frac{1}{v} \left( \dot{q}_c + \frac{P}{A} \cdot \dot{q}_s \right). \]

The steady-state solution for the coolant concentration is then

\[
C(x) = C(0) + \frac{\dot{q}_c + \frac{P}{A} \cdot \dot{q}_s}{v} x. \quad (91)
\]

This solution is independent of the relationship \( B = f(S) \). This is because in the steady-state the mass flux through the boundary layer
depends only on the plateout source rate (Eq. (90)) and not on the surface concentration. The surface concentration $S$, however, does depend on $B(S)$. Eq. (90) gives

$$B(x) = \frac{q_S}{h} + C(x),$$

from which $S(x)$ can be computed. If we assume for $B$ a functional relationship of the form

$$B = \alpha + \beta S^\gamma,$$  \hspace{1cm} (92)

then

$$S(x) = \left(\frac{B-\alpha}{\beta}\right)^{1/\gamma} = \left\{\frac{\dot{q}_s + h[C(x)-\alpha]}{h \beta}\right\}^{1/\gamma}.$$ \hspace{1cm} (93)

PADLOC considers three special cases for the sorption behavior.

a. $\alpha \neq 0$, $\beta \neq 0$, $\gamma = 1$; general linear case

$$S(x) = \frac{\dot{q}_s + h[C(x)-\alpha]}{h \beta}$$ \hspace{1cm} (94)

b. $\alpha = 0$, $\beta \neq 0$, $\gamma = 1$; Langmuir sorption

$$S(x) = \frac{\dot{q}_s + h C(x)}{h \beta}$$ \hspace{1cm} (95)

c. $\alpha = 0$, $\beta \neq 0$, $\gamma > 1$; Freundlich sorption

$$S(x) = \left[\frac{\dot{q}_s + h C(x)}{h \beta}\right]^{1/\gamma}.$$ \hspace{1cm} (96)
We now turn to a decaying species for which \( \lambda \neq 0 \). In order to render the solution analytically tractable we will restrict ourselves to the linear sorption case \( (\gamma = 1) \), i.e.,

\[ B = \alpha + \beta S . \tag{97} \]

Substituting (97) into (89) one obtains

\[ S(x) = \frac{q_s + h[C(x) - \alpha]}{\lambda + h \beta} . \tag{98} \]

Substituting (97) and (98) into (88) and eliminating \( B \) gives

\[ \frac{dC(x)}{dx} + \omega C(x) = Q' , \tag{99} \]

where

\[ \omega = \frac{1}{\nu} \left[ \lambda + \frac{p}{A} h \left( 1 - \frac{h \beta}{\lambda + h \beta} \right) \right] , \tag{100} \]

and

\[ Q' = \frac{1}{\nu} \left[ \frac{q_s}{\gamma} + \frac{p}{A} h \left( \alpha + \beta \frac{\dot{q}_s - h \alpha}{\lambda + h \beta} \right) \right] . \tag{101} \]

Eq. (99) has the solution

\[ C(x) = C(0) e^{-\omega x} + \frac{Q'}{\omega} \left( 1 - e^{-\omega x} \right) . \tag{102} \]

PADLOC has also the capability of considering either sorption only or desorption only of the plateout surface. The former case is characterized by \( C \gg B \) and the latter by \( B \gg C \). Also, for desorption only, any surface source rate flux is directly transmitted to the coolant where it appears as a coolant source rate.
The solutions for adsorption only and desorption only can be obtained by substituting appropriate limiting values for (B-C) in the system (88), (89). The results are given below.

a. Adsorption only (C >> B)

\[ C_A(x) = C_A(0) e^{-\omega_A x} + \frac{Q_A^*}{\omega_A} \left( 1 - e^{-\omega_A x} \right), \]

\[ S_A(x) = \frac{1}{\lambda} \left[ q_s + h C_A(x) \right], \]

where

\[ \omega_A = \frac{1}{\lambda} \left( \lambda + \frac{P}{A} h \right), \]

and

\[ Q_A^* = \frac{q_c}{v^\prime}. \]

b. Desorption only (B >> C)

\[ C_D(x) = C_D(0) e^{-\omega_D x} + \frac{Q_D^*}{\omega_D} \left( 1 - e^{-\omega_D x} \right), \]

\[ S_D(x) = 0, \]

where

\[ \omega_D = \frac{\lambda}{v^\prime}, \]

and

\[ Q_D^* = \frac{1}{v^\prime} \left( \frac{q_c}{q_s} + \frac{P}{A} q_s \right). \]

* The subscripts A and D stand for adsorption and desorption.
7.3 COMPARISON OF PADLOC RESULTS WITH HAND CALCULATIONS

7.3.1 Introduction

The following sample problems exhibit some of the PADLOC capabilities. The values of certain input parameters are chosen in such a way that related physical effects show up clearly in the results. These include temperature and pressure discontinuities at branch connections, decay constants, and sorption parameters. Some of the parameters, e.g., temperature discontinuities, may not be physically meaningful.

For each case considered the results of PADLOC are compared with hand calculations, employing the analytic solutions derived in the previous section.

7.3.2 Examples

7.3.2.1 Verification of Time Dependence, Example 1

We consider a decaying nuclide in a closed loop with uniform parameters. As previously indicated, the coolant and plateout concentrations in such a loop are independent of the spatial distance \( x \) and depend only on the time \( t \).

In PADLOC the minimum number of branches allowed for a closed loop is two. We will thus employ a two-branch network as shown in the sketch.

![Diagram of a two-branch network](image)
The PADLOC input parameters for both branches are the same. They are assumed to be:

- **branch length**: \( L = 10 \text{ cm} \)
- **hydraulic diameter (circular cross section)**: \( d = 2 \text{ cm} \)
- **forced convection**: \( \text{KGF} = 1 \)
- **mesh spacing**: \( \Delta x = 5 \text{ cm} \)
- **initial coolant concentration**: \( C(o) = 0 \)
- **initial surface concentration**: \( S(o) = 0 \)
- **decay constant**: \( \lambda = 10 \text{ 1/sec} \)
- **helium mass flow rate**: \( \dot{m} = 42.0855 \text{ g/sec} \)
- **coolant and wall temperature**: \( T = 800^\circ\text{C} \)
- **coolant pressure**: \( p = 50 \text{ atm} \)
- **coolant source rate**: \( \dot{q}_c = 0 \)
- **surface source rate**: \( \dot{q}_s = 2.2\times10^7 \text{ atoms/cm}^2\text{sec} \)

The sorption behavior is to be "linear with saturation" (LS) according to Eqs. (64) and (65) on page 66. The sorption constants are chosen to be

\[
S = 10^{20} \text{ atoms/cm}^2 \quad \text{(surface saturation concentration)}
\]
\[
AVPOR = 3.88
\]
\[
BVPOR = 3.73 \times 10^{30} \text{K}
\]

**Results**

Various time steps \( \Delta t \) and time integration parameters \( \theta \) were used to generate PADLOC results. For comparison, hand calculations for the coolant and plateout concentrations were based on Eqs.(87), (74), and (77) on pages 89 and 88. The sorption parameters \( \alpha \) and \( \beta \) in these equations were computed using Eqs.(64) and (65) together with above sorption constants. For the mass transfer coefficient \( h \) appropriate relations of Appendix A (Eq. (A1), page 1-A, Table A1, page 3-A) were used. Figure 6 on the following page shows the time dependence of the coolant concentration \( C \) and surface concentration \( S \) based on the hand calculations.* In Figure 7 (page 97),

* The details are preserved in Ref. 4.
Fig. 6. Example 1: Time dependence of the coolant and plateout concentrations
Fig. 7. Example 1: Relative error (%) of coolant concentration versus time
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<th>Time [sec]</th>
<th>C [atoms/cm^3]</th>
<th>S [atoms/cm^2]</th>
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<th>ε_s [%]</th>
<th>ε_c [%]</th>
<th>ε_s [%]</th>
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<td>-0.23</td>
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<td>0.07</td>
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<td>3.938+5</td>
<td>-1.34</td>
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<td>1.39</td>
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Figure 8, Example 1
PADLOC Printout for $t = 0.05$ sec ($\theta = 0.5$, $\Delta t = 5 \times 10^{-4}$ sec)

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<td>HE MASS FLOW RATE</td>
<td>$4.208550+01$ G/S</td>
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<table>
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<tr>
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<th>FLUORATE MOL/S</th>
<th>BULK C A/CCM</th>
<th>SOURCE RTE MOL/S A/(SCM*S)</th>
<th>CONDUIT CROSS CM</th>
<th>M,TRANSF TEMP PRESS VELOC CM/S</th>
<th>HE-COOLANT MOL/S A/(SCM*S)</th>
<th>PRESS</th>
<th>CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
<tr>
<td>2</td>
<td>5.000000</td>
<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
<tr>
<td>3</td>
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<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>STEP</th>
<th>1.100000+02</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME</td>
<td>$4.999998+02$ s, $1.000000+02$ TIME STEPS, DELTAT $5.000000+04$ s, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK 0</td>
</tr>
<tr>
<td>HE MASS FLOW RATE</td>
<td>$4.208550+01$ G/S</td>
</tr>
<tr>
<td>BRANCH TOTAL POINTS, BEGIN 2, END 1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>DE</th>
<th>DIST. CM</th>
<th>FLUORATE MOL/S</th>
<th>BULK C A/CCM</th>
<th>SOURCE RTE MOL/S A/(SCM*S)</th>
<th>CONDUIT CROSS CM</th>
<th>M,TRANSF TEMP PRESS VELOC CM/S</th>
<th>HE-COOLANT MOL/S A/(SCM*S)</th>
<th>PRESS</th>
<th>CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
<tr>
<td>2</td>
<td>5.000000</td>
<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
<tr>
<td>3</td>
<td>1.000000</td>
<td>$1.403333+01$</td>
<td>$4.413+04$</td>
<td>$-8.543+05$</td>
<td>$8.436+05$</td>
<td>0.000</td>
<td>$2.200+07$</td>
<td>3.142+00</td>
<td>6.283+00</td>
</tr>
</tbody>
</table>
the relative errors of PADLOC results are plotted vs. time. For a time step of $\Delta t = 5 \times 10^{-4}$ s and Crank Nicholson time integration ($\theta = 0.5$), the PADLOC error is zero. For $\theta \neq 0.5$ and/or larger time steps, errors are largest at the end of the first time step. Table 1 on page 98 gives detailed numerical values. Figure 8 is a PADLOC printout for $T = 0.05$ s ($\theta = 0.5$, $\Delta t = 5 \times 10^{-4}$ s).

7.3.2.2 Verification of Spatial Dependence

In this section the steady-state PADLOC results will be compared with hand calculations. Various networks, flow conditions, decay constants, and sorption behaviors will be employed.

a. Example 2, Simulation of a LOFC Accident

Consider the following network of seven branches and seven global nodal points. With the exception of branch 6, which has been added to demonstrate a boundary condition, this network is identical to the one of Figure 4 (p. 9) for an

```
1 4 7
branch 1 branch 3

2 6 3
branch 2 branch 4

5
branch 5
branch 6

10^{-15} \text{ mol/sec (boundary condition)}
```
LOFC accident. Branch 2 represents the core and branches 4 and 5 the circulators and steam generators. Global point 4 represents the relief valve (for branch 1) in the upper plenum, and branches 1 and 3 are flow paths in the containment building. To simulate an LOFC accident we assume the coolant flow in branch 1 to be zero for the first 7 time points (closed relief valve) and to be greater than zero for time points IT > 8 (the relief valve opens at IT = 8). At global point 2 the incoming fission product flow rate is to be 10^{-15} mol/sec. The fission product being considered is stable with λ=0. Table 2 on the following page shows pertinent branch dependent PADLOC input. The sorption behavior is to be "linear with saturation" (LS) for branch 1 and Freundlich (F) for branches two through seven. The sorption constants are assumed to be

\begin{align*}
\text{LS:} & \quad \text{AVPOR} = 3.88 \\
& \quad \text{BVPOR} = 3.73 \times 10^{3°K} \\
& \quad S_S = 10^{20} \text{ atoms/cm}^2 \\
\text{See Eqs. (64) and (65), page 66.}
\end{align*}

\begin{align*}
\text{F:} & \quad \text{ACP} = 1 \\
& \quad \text{BCP} = 900°K \\
& \quad \text{DCP} = 1°K \\
& \quad \text{CCP} = 3600 \\
\text{See Eq. (66), page 67.}
\end{align*}

**Hand Calculations**

The basic equations to be used for determining the steady-state coolant and plateout concentrations are Eqs.(91) and (93). For a stable nuclide,

\[
C(x) = C(o) + \frac{q_c + \frac{P}{A} q_s}{v} x ,
\]

\[
S(x) = \left(\frac{q_s + h[C(x) - \alpha]}{h \beta}\right)^{1/Y}.
\]
### Table 2

**Example 2**

Branch Dependent PADLOC Input

<table>
<thead>
<tr>
<th>Branch</th>
<th>Time Point IT</th>
<th>Length L [cm]</th>
<th>Mesh Spacing Δx [cm]</th>
<th>Hydraulic Diam. d [cm]</th>
<th>Coolant Flow Rate ( \dot{m} ) [g/s]</th>
<th>Coolant Pressure ( p ) [at]</th>
<th>Coolant and Wall Temp T[°C]</th>
<th>Sorption* Behavior</th>
<th>Coolant Source Rate ( q_c ) [atoms cm(^{-2}) s(^{-1})]</th>
<th>Surface Source Rate ( q_s ) [atoms cm(^{-2}) s(^{-1})]</th>
<th>Initial Concentrations**</th>
<th>Forced Convection in Pipe of Circular Cross Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(&lt; 7)</td>
<td>10</td>
<td>5</td>
<td>1</td>
<td>0</td>
<td>30</td>
<td>500</td>
<td>LS</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>2</td>
<td>(\geq 1)</td>
<td>10</td>
<td>5</td>
<td>2</td>
<td>42.0855</td>
<td>50</td>
<td>800</td>
<td>F</td>
<td>0</td>
<td>2.2\times10^7</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>3</td>
<td>(&lt; 7)</td>
<td>10</td>
<td>5</td>
<td>3</td>
<td>30</td>
<td>30</td>
<td>500</td>
<td>F</td>
<td>0</td>
<td>5\times10^7</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>4</td>
<td>(\geq 1)</td>
<td>10</td>
<td>5</td>
<td>4</td>
<td>12.0855</td>
<td>40</td>
<td>750</td>
<td>F*</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>5</td>
<td>(\geq 1)</td>
<td>10</td>
<td>5</td>
<td>5</td>
<td>12.0855</td>
<td>30</td>
<td>700</td>
<td>F</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>(\geq 1)</td>
<td>10</td>
<td>5</td>
<td>6</td>
<td>30</td>
<td>30</td>
<td>500</td>
<td>F</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Yes</td>
</tr>
<tr>
<td>7</td>
<td>(\geq 1)</td>
<td>10</td>
<td>5</td>
<td>7</td>
<td>30</td>
<td>30</td>
<td>750</td>
<td>F</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Yes</td>
</tr>
</tbody>
</table>

* LS = Linear with saturation.
  F = Freundlich.

** \( C(o,x) \), \( S(o,x) \).
where $\alpha$, $\beta$, and $\gamma$ are the sorption constants in the sorption relation

$$B(S) = \alpha(T) + \beta(T) S^\gamma(T).$$

From these equations it follows that the steady-state concentrations depend on the inlet coolant concentration $C(o)$ and on the source rates $\dot{q}_c$ and $\dot{q}_s$. For zero sources (branches 1, 4, 5, 6, 7) the concentrations are independent of $x$. For non-zero sources (branches 2 and 3) the $x$-dependence is linear.

To determine the branch inlet coolant concentrations for the network, it is convenient to use fission product flow rates $\dot{M}$. The flow rates are

$$\dot{M}_i(x) = \frac{v_i A_i}{N_A} C_i(x), \quad \text{g mole/sec}$$

where

- $i =$ branch index,
- $v_i =$ coolant velocity,
- $A_i =$ conduit cross section area,
- $N_A =$ Avogadro's number.

Known flow rates can then be converted back to coolant concentrations. We will now demonstrate how the inlet flow rates can be found by hand calculation. Employing the mixing equations of Section 5.3 (p. 39), we set up a system of equations similar to the global system employed by PADLOC:
\[ \dot{M}_1 = \frac{m_1}{m_7} \] branch 1

\[ \dot{M}_2(o) = \dot{M}_5 + \dot{M}_6 \]

\[ \dot{M}_2(L_2) = \dot{M}_2(o) + \left( \frac{\dot{q}_c + \frac{P}{A} \dot{q}_s}{v} \right) \frac{v_2 A_2}{N_A} L_2 \] branch 2

\[ \dot{M}_3(o) = \frac{m_3}{m_7} \dot{M}_7 \] branch 3

\[ \dot{M}_4 = \frac{m_4}{m_2} \dot{M}_2(L_2) \] branch 4

\[ \dot{M}_5 = \dot{M}_4 \] branch 5

\[ \dot{M}_6 = 10^{-15} \text{ mol/s (boundary condition)} \] branch 6

\[ \dot{M}_7 = \frac{m_7}{m_2} \dot{M}_2(L_2) \] branch 7

It is noted that no x-dependence is shown for the fission product flow rates of branches with zero sources.

After solving the above system for the branch inlet mass flow rates, branch concentrations can be computed using the equations for C(x) and S(x) shown on page 101. The values for the sorption parameters \( \alpha, \beta, \text{ and } \gamma \) can be obtained from Eqs. (64), (65), and (66) for LS and F sorption behaviors. The coolant velocities can be calculated according to
Eq. (A9) of Appendix A. For the mass transfer coefficients $h$ appropriate relations for forced convection in circular tubes (Eq. (A1) and Table A1 of Appendix A) can be used.

Table 3 on the following page gives the results of the hand calculations.* For comparison, Figures 9 and 10 (pp. 107, 111) show the steady state PADLOC printouts. It is noted that the PADLOC results are in exact agreement with the hand calculations of Table 3.

b. Example 3, Flow Reversals

The network for this problem is the same as for the previous example. To simplify the hand calculations the plateout source rate in branch 3 is now set to zero, and we assume "linear with saturation" (LS) sorption behavior for all branches. The assumed coolant flow rates for the different branches are shown in Figure 11 on page 115. It can be seen that the flows in branches 2, 4, and 5 are simultaneously reversed at time $t = 15$ min and that the original flow directions are reestablished at $t = 26$ min. Otherwise the conditions are the same as for Example 2.

We again use fission product mass flow rates to calculate branch inlet conditions and use Eqs. (91) and (93) later to compute concentrations in the branches. The global equations for positive coolant flows in all branches are the same as for Example 2 with one exception. Since the source rate in branch 3 is now zero, the mixing equation

$$\dot{M}_3(0) = \frac{m_3}{m_7} \dot{M}_7$$

is replaced by

$$\dot{M}_3 = \frac{m_3}{m_7} \dot{M}_7.$$

* The details are presented in Ref. 4.
Table 3
Example 2
Results of Hand Calculations
Steady-State Values of Fission Product Flow Rates $\dot{M}$, Coolant Concentrations $C$, and Plateout Concentrations $S$

<table>
<thead>
<tr>
<th>Branch</th>
<th>$\dot{M}$ [mol/sec]</th>
<th>$C$ [atoms/cm$^3$]</th>
<th>$S$ [atoms/cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 IT$&lt;7$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IT$&gt;8$</td>
<td>2.197E-15</td>
<td>1.211E+5</td>
<td>1.160E+7</td>
</tr>
<tr>
<td>2</td>
<td>$x=0$ cm</td>
<td>2.328E-15</td>
<td>7.321E+4</td>
</tr>
<tr>
<td>$x=5$ cm</td>
<td>3.475E-15</td>
<td>1.093E+5</td>
<td>9.300E-4</td>
</tr>
<tr>
<td>$x=10$ cm</td>
<td>4.623E-15</td>
<td>1.454E+5</td>
<td>9.330E-4</td>
</tr>
<tr>
<td>3</td>
<td>$x=0$ cm</td>
<td>3.295E-15</td>
<td>1.211E+5</td>
</tr>
<tr>
<td>$x=5$ cm</td>
<td>7.208E-15</td>
<td>2.649E+5</td>
<td>5.533E-3</td>
</tr>
<tr>
<td>$x=10$ cm</td>
<td>1.112E-14</td>
<td>4.086E+5</td>
<td>5.543E-3</td>
</tr>
<tr>
<td>IT$&gt;8$</td>
<td>$x=0$ cm</td>
<td>1.098E-15</td>
<td>1.211E+5</td>
</tr>
<tr>
<td>$x=5$ cm</td>
<td>5.011E-15</td>
<td>5.524E+5</td>
<td>6.460E-3</td>
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<tr>
<td>$x=10$ cm</td>
<td>8.928E-15</td>
<td>9.837E+5</td>
<td>6.475E-3</td>
</tr>
<tr>
<td>4</td>
<td>1.328E-15</td>
<td>1.220E+5</td>
<td>5.959E-4</td>
</tr>
<tr>
<td>5</td>
<td>1.328E-15</td>
<td>9.620E+4</td>
<td>7.387E-4</td>
</tr>
<tr>
<td>6</td>
<td>1.000E-15</td>
<td>3.675E+4</td>
<td>1.942E-3</td>
</tr>
<tr>
<td>7</td>
<td>3.295E-15</td>
<td>9.150E+4</td>
<td>5.592E-4</td>
</tr>
</tbody>
</table>
### Figure 9, Example 2

Steady-state PADLOC results \( (t = 6 \text{ sec}) \)
Zero coolant flow in Branch 1 \( (\theta=1, \Delta t=1 \text{ sec}) \)

<table>
<thead>
<tr>
<th>Branch 1, No Sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME = 6.000000<em>00 s, 6.000000</em>00 TIME STEPS, DELTAT = 1.000000*00 s, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK = 1</td>
</tr>
<tr>
<td>HE MASS FLOW RATE = 0.000000 G/S</td>
</tr>
<tr>
<td>Branch Global Points, Begin 4, End 1</td>
</tr>
</tbody>
</table>

```
|   |       |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 1 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 7.854-01 | 3.142*00 | 500. | 500. | 30. | 6.263*00 |
| 2 | 5.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 7.854-01 | 3.142*00 | 500. | 500. | 30. | 6.283*00 |
| 3 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 7.854-01 | 3.142*00 | 500. | 500. | 30. | 6.283*00 |
```

### Branch 2, Plateout Region Source = 2.2E7 ATOMS/(S*CM**2)

| TIME = 6.000000*00 s, 6.000000*00 TIME STEPS, DELTAT = 1.000000*00 s, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK = 1 |
| HE MASS FLOW RATE = 4.208550*01 G/S |
| Branch Global Points, Begin 5, End 6 |

```
|   |       |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 1 | 0.000 | 2.328-15 | 7.321*04 | -2.200*07 | 9.271-04 | 0.000 | 2.200*07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
| 2 | 5.000 | 3.475-15 | 1.093*05 | -2.200*07 | 9.300-04 | 0.000 | 2.200*07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
| 3 | 1.000 | 4.623-15 | 1.454*05 | -2.200*07 | 9.330-04 | 0.000 | 2.200*07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
```
### Branch 3

- **Time:** 6.000000*00 s, 6.000000*00 time steps, **Delta T:** 1.000000*00 s, **Number of iterations for the total network:** 1
- **He Mass flow rate:** 3.000000*01 g/s
- **Branch Global Points:** BEGIN 4, END 7

<table>
<thead>
<tr>
<th><strong>Dist.</strong></th>
<th><strong>Flume</strong></th>
<th><strong>Bulk Flux</strong></th>
<th><strong>Plate</strong></th>
<th><strong>Source RTE</strong></th>
<th><strong>Conduit</strong></th>
<th><strong>He-Coolant</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>3.295-15</td>
<td>1.211*05</td>
<td>-5.000*07</td>
<td>5.523-03</td>
<td>0.000</td>
<td>5.000*07</td>
</tr>
<tr>
<td>5.000*00</td>
<td>7.208-15</td>
<td>2.669*05</td>
<td>-5.000*07</td>
<td>5.533-03</td>
<td>0.000</td>
<td>5.000*07</td>
</tr>
<tr>
<td>1.000*01</td>
<td>1.112-14</td>
<td>4.086*05</td>
<td>-5.000*07</td>
<td>5.543-03</td>
<td>0.000</td>
<td>5.000*07</td>
</tr>
</tbody>
</table>

### Branch 4

- **Time:** 6.000000*00 s, 6.000000*00 time steps, **Delta T:** 1.000000*00 s, **Number of iterations for the total network:** 1
- **He Mass flow rate:** 1.208550*01 g/s
- **Branch Global Points:** BEGIN 6, END 3

<table>
<thead>
<tr>
<th><strong>Dist.</strong></th>
<th><strong>Flume</strong></th>
<th><strong>Bulk Flux</strong></th>
<th><strong>Plate</strong></th>
<th><strong>Source RTE</strong></th>
<th><strong>Conduit</strong></th>
<th><strong>He-Coolant</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>1.328-15</td>
<td>1.220*05</td>
<td>1.503-02</td>
<td>5.959-04</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5.000*00</td>
<td>1.328-15</td>
<td>1.220*05</td>
<td>1.288-02</td>
<td>5.959-04</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1.000*01</td>
<td>1.328-15</td>
<td>1.220*05</td>
<td>0.000</td>
<td>5.959-04</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

### Branch 5

- **Time:** 6.000000*00 s, 6.000000*00 time steps, **Delta T:** 1.000000*00 s, **Number of iterations for the total network:** 1
- **He Mass flow rate:** 1.208550*01 g/s
- **Branch Global Points:** BEGIN 3, END 5
### HE-COOLANT Conduit

<table>
<thead>
<tr>
<th>NDE</th>
<th>CM</th>
<th>MOL/S</th>
<th>A/CCM</th>
<th>A/(SCM*S)</th>
<th>A/SCM</th>
<th>A/(CCM*S)</th>
<th>SCM</th>
<th>CM</th>
<th>C</th>
<th>C</th>
<th>ATM</th>
<th>CM/S</th>
<th>CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>1.087-02</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
</tr>
<tr>
<td>2</td>
<td>5.000+00</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>9.056-03</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
</tr>
<tr>
<td>3</td>
<td>1.000+01</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>8.151-03</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
</tr>
</tbody>
</table>

### HE-COOLANT

**ATOM BULK FLUX PLATE**

**SOURCE**

**RTE**

**CROSS WALL**

**DIST.**

**FLORTE**

**C C TO P OUT C COOL. PLTOUT SECT. PERIM TEMP TEMP PRESS VELOC COEFF**

**NOE CM MOL/S A/CCM A/(SCM*S) A/SCM A/(CCM*S)**

<table>
<thead>
<tr>
<th>NDE</th>
<th>CM</th>
<th>MOL/S</th>
<th>A/CCM</th>
<th>A/(SCM*S)</th>
<th>A/SCM</th>
<th>A/(CCM*S)</th>
<th>SCM</th>
<th>CM</th>
<th>C</th>
<th>C</th>
<th>ATM</th>
<th>CM/S</th>
<th>CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>4.698-03</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>5.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>1.000+00</td>
</tr>
<tr>
<td>2</td>
<td>5.000+00</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>8.264-03</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>5.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>1.000+00</td>
</tr>
<tr>
<td>3</td>
<td>1.000+01</td>
<td>1.328-15</td>
<td>3.675+04</td>
<td>5.220-03</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>5.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>1.000+00</td>
</tr>
</tbody>
</table>

---

**BRANCH 6, NO SOURCES, BOUNDARY CONDITION AT END POINT 2 IS 1.E-15 MOLES/S**

**TIME: 6.000000*00 S, 6.000000*00 TIME STEPS, DELTAT: 1.000000*00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 1**

**HE MASS FLOW RATE: 3.000000+01 G/S**

**BRANCH GLOBAL POINTS, BEGIN 2, END 5**

---

**BRANCH 7, NO SOURCES**

**TIME: 6.000000*00 S, 6.000000*00 TIME STEPS, DELTAT: 1.000000*00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 1**

**HE MASS FLOW RATE: 3.000000+01 G/S**

**BRANCH GLOBAL POINTS, BEGIN 6, END 4**

---
Figure 10, Example 2

Steady-state PADLOC results (t = 60 sec)
Non-zero coolant flows in all branches (δ=1, Δt=1 sec)

<table>
<thead>
<tr>
<th>STEP o.000000+01</th>
<th>STEP o.000000+01</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. <strong>BRANCH 1, NO SOURCES</strong></td>
<td></td>
</tr>
<tr>
<td>TIME: 6.000000+01 S, 6.000000+01 TIME STEPS, DELTAT: 1.000000+00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 1</td>
<td></td>
</tr>
<tr>
<td>HE MASS FLOW RATE: 2.000000+01 G/S</td>
<td></td>
</tr>
<tr>
<td>BRANCH GLOBAL POINTS, BEGIN 4, END 1</td>
<td></td>
</tr>
<tr>
<td>HE-COOLANT</td>
<td>HE-COOLANT</td>
</tr>
<tr>
<td>ATOM</td>
<td>BULK</td>
</tr>
<tr>
<td>DIST.</td>
<td>FLORTE</td>
</tr>
<tr>
<td>NDE</td>
<td>CM</td>
</tr>
<tr>
<td>1</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>5.000+00</td>
</tr>
<tr>
<td>3</td>
<td>1.000+01</td>
</tr>
</tbody>
</table>

| 2. **BRANCH 2, PLATEOUT REGION SOURCE = 2.2E7 ATOMS/(S*CM**2) |
| TIME: 6.000000+01 S, 6.000000+01 TIME STEPS, DELTAT: 1.000000+00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 1 |
| HE MASS FLOW RATE: 4.208550+01 G/S |
| BRANCH GLOBAL POINTS, BEGIN 5, END 6 |
| HE-COOLANT | HE-COOLANT | HE-COOLANT |
| ATOM | BULK | FLUX | PLATE | CROSS | WALL | CONDUIT | HE-COOLANT | M.TRNSF |
| DIST. | FLORTE | C | C TO P | OUT C | SECT. | PERIM | TEMP | TEMP | PRESS | VELOC | COEFF |
| NDE | CM | MOL/S | A/CCM | A/(SCM*S) | A/SCM | A/(CCM*S) | A/(SCM*S) | SCM | CM | C | ATM | CM/S | CM/S |
| 1 | 0.000 | 2.326-15 | 7.321+04 | -2.200+07 | 9.271-04 | 0.000 | 2.200+07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
| 2 | 5.000+00 | 3.475-15 | 1.093+05 | -2.200+07 | 9.300-04 | 0.000 | 2.200+07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
| 3 | 1.000+01 | 4.623-15 | 1.454+05 | -2.200+07 | 9.330-04 | 0.000 | 2.200+07 | 3.142+00 | 6.283+00 | 800. | 800. | 50. | 6.095+03 | 8.763+00 |
The page contains detailed information about the thermal hydraulic behavior of a system, likely from a computer simulation or analysis report. It includes sections on branch points, mass flow rates, and various thermal properties such as temperatures, pressures, and velocities. The data is presented in a structured format with tables and numerical values, indicating the flow and characteristics of different branches of the system over time.

For instance, Branch 3 has a mass flow rate of 1.000000+01 G/S, with parameters such as the number of iterations and global points for the total network. The tables show the flux, temperature, and other properties at different points, providing a comprehensive overview of the thermal behavior across the system.
<table>
<thead>
<tr>
<th>DIST. CM</th>
<th>FLORE C CM</th>
<th>BULK FLO X A/CM</th>
<th>FLUX X A/(SCM*S)</th>
<th>PLATE X A/SCM</th>
<th>COOL. X A/(CCM*S)</th>
<th>RTE X A/(SCM*S)</th>
<th>CROSS X SCM</th>
<th>PERIM X CM</th>
<th>TEMP X C</th>
<th>TEMP X ATM</th>
<th>PRESS X CM/S</th>
<th>VELOC X CM/S</th>
<th>COEFF X CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.000</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>0.000</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
<td>9.274-01</td>
</tr>
<tr>
<td>2 5.000+00</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>0.000</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
<td>9.274-01</td>
</tr>
<tr>
<td>3 1.000+01</td>
<td>1.328-15</td>
<td>9.620+04</td>
<td>0.000</td>
<td>7.387-04</td>
<td>0.000</td>
<td>0.000</td>
<td>1.963+01</td>
<td>1.571+01</td>
<td>700.</td>
<td>700.</td>
<td>30.</td>
<td>4.232+02</td>
<td>9.274-01</td>
</tr>
</tbody>
</table>

-- Branch 6 --

TIME = 6.000000+01 S, 6.000000+01 TIME STEPS, DELTAT = 1.000000+00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK = 1
HE MASS FLOW RATE = 3.000000+01 G/S
BRANCH GLOBAL POINTS, BEGIN 2, END 5

<table>
<thead>
<tr>
<th>DIST. CM</th>
<th>FLORE C CM</th>
<th>BULK FLO X A/CM</th>
<th>FLUX X A/(SCM*S)</th>
<th>PLATE X A/SCM</th>
<th>COOL. X A/(CCM*S)</th>
<th>RTE X A/(SCM*S)</th>
<th>CROSS X SCM</th>
<th>PERIM X CM</th>
<th>TEMP X C</th>
<th>TEMP X ATM</th>
<th>PRESS X CM/S</th>
<th>VELOC X CM/S</th>
<th>COEFF X CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.000</td>
<td>1.000-15</td>
<td>3.675+04</td>
<td>4.698-03</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>2.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>5.796+02</td>
<td>1.069+00</td>
</tr>
<tr>
<td>2 5.000+00</td>
<td>1.000-15</td>
<td>3.675+04</td>
<td>0.000</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>2.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>5.796+02</td>
<td>1.069+00</td>
</tr>
<tr>
<td>3 1.000+01</td>
<td>1.000-15</td>
<td>3.675+04</td>
<td>0.000</td>
<td>1.942-03</td>
<td>0.000</td>
<td>0.000</td>
<td>2.827+01</td>
<td>1.885+01</td>
<td>500.</td>
<td>500.</td>
<td>30.</td>
<td>5.796+02</td>
<td>1.069+00</td>
</tr>
</tbody>
</table>

-- Branch 7 --

TIME = 6.000000+01 S, 6.000000+01 TIME STEPS, DELTAT = 1.000000+00 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK = 1
HE MASS FLOW RATE = 3.000000+01 G/S
BRANCH GLOBAL POINTS, BEGIN 6, END 4

<table>
<thead>
<tr>
<th>DIST. CM</th>
<th>FLORE C CM</th>
<th>BULK FLO X A/CM</th>
<th>FLUX X A/(SCM*S)</th>
<th>PLATE X A/SCM</th>
<th>COOL. X A/(CCM*S)</th>
<th>RTE X A/(SCM*S)</th>
<th>CROSS X SCM</th>
<th>PERIM X CM</th>
<th>TEMP X C</th>
<th>TEMP X ATM</th>
<th>PRESS X CM/S</th>
<th>VELOC X CM/S</th>
<th>COEFF X CM/S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.000</td>
<td>3.295-15</td>
<td>9.150+04</td>
<td>9.736-03</td>
<td>5.592-04</td>
<td>0.000</td>
<td>0.000</td>
<td>3.848+01</td>
<td>2.199+01</td>
<td>750.</td>
<td>750.</td>
<td>30.</td>
<td>5.636+02</td>
<td>1.108+00</td>
</tr>
<tr>
<td>2 5.000+00</td>
<td>3.295-15</td>
<td>9.150+04</td>
<td>0.000</td>
<td>5.592-04</td>
<td>0.000</td>
<td>0.000</td>
<td>3.848+01</td>
<td>2.199+01</td>
<td>750.</td>
<td>750.</td>
<td>30.</td>
<td>5.636+02</td>
<td>1.108+00</td>
</tr>
<tr>
<td>Value1</td>
<td>Value2</td>
<td>Value3</td>
<td>Value4</td>
<td>Value5</td>
<td>Value6</td>
<td>Value7</td>
<td>Value8</td>
<td>Value9</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.1000E+01</td>
<td>3.295-15</td>
<td>9.150+04</td>
<td>0.000</td>
<td>5.592-04</td>
<td>0.000</td>
<td>0.000</td>
<td>3.648+01</td>
<td>2.199+01</td>
<td>750.</td>
<td>750.</td>
<td>30.</td>
<td>5.636+02</td>
<td>1.108+00</td>
</tr>
</tbody>
</table>
Fig. 11. Example 3: Coolant flow rates
After changing the flow directions in branches 2, 4 and 5, the fission product flow rates in these branches become negative too. For the mixing equations, however, we will use absolute values of these flow rates. The reason for this was discussed in Section 5.5. The global system is then

\[
\begin{align*}
\dot{M}_1 &= \frac{m_1}{m_7} \dot{M}_7 \\
|\dot{M}_2(L_2)| &= \frac{m_2}{m_4} |\dot{M}_4| \\
|\dot{M}_2(o)| &= |\dot{M}_2(L_2)| + \left(\frac{q_c + \frac{p}{A} q_s}{v} \right) \frac{v_2 A_2}{N_A} L_2 \\
\dot{M}_3 &= \frac{m_3}{m_7} \dot{M}_7 \\
|\dot{M}_4| &= |\dot{M}_5| \\
|\dot{M}_5| &= |\dot{M}_2(o)| + M_6 \\
\dot{M}_6 &= 10^{-15} \text{ mol/s} \\
\dot{M}_7 &= \frac{m_7}{m_4} |\dot{M}_4|
\end{align*}
\]

branch 1

branch 2

branch 3

branch 4

branch 5

branch 6

branch 7
We can now solve for these flow rates as before and compute the coolant and plateout concentrations using Eqs. (91) and (93). The results are given in Table 4 on the following page.* Since branch 2 is the only branch containing a source term, only the concentrations of this branch are affected by the flow reversals. Figure 12 on page 119 shows the time dependence of the branch concentrations of the corresponding PADLOC run. Figures 13 and 14 (pp. 120, 123) show steady-state PADLOC results for $t = 25$ min and $t = 40$ min. As can be seen the PADLOC results are in exact agreement with the results of the hand calculations of Table 4.

**c. Example 4, Closed Loop**

In this problem we consider a decaying fission product in a closed loop consisting of two branches as shown below. Branch 2 has a surface source rate of $2.2 \times 10^7$ atoms/$(cm^2 \cdot sec)$. We again assume "linear with saturation" (LS) sorption behavior for both branches. After steady-state conditions are reached, flows are reversed. Pertinent PADLOC input is shown on page 127.

* The details are found in Ref. 4.
Table 4

Example 3

Steady-State Values of Fission Product Flow Rates $\dot{M}$, Coolant Concentrations $C$, and Plateout Concentrations $S$

<table>
<thead>
<tr>
<th>Branch</th>
<th>All Coolant Flow Rates Positive</th>
<th>Negative Coolant Flow Rates in Branches 2, 4 and 5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\dot{M}$ [mol/s]</td>
<td>$C$ [atoms/cm$^3$]</td>
</tr>
<tr>
<td>1</td>
<td>2.197-15</td>
<td>1.211+5</td>
</tr>
<tr>
<td></td>
<td>3.475-15</td>
<td>1.093+5</td>
</tr>
<tr>
<td></td>
<td>4.623-15</td>
<td>1.454+5</td>
</tr>
<tr>
<td>3</td>
<td>1.098-15</td>
<td>1.211+5</td>
</tr>
<tr>
<td>4</td>
<td>1.328-15</td>
<td>1.220+5</td>
</tr>
<tr>
<td>6</td>
<td>1.000-15</td>
<td>3.675+4</td>
</tr>
</tbody>
</table>
Fig. 12. Example 3: Coolant concentrations (atoms/cm\(^3\)) at branch points \(x = 0\) versus time
**Figure 13, Example 3**

Steady-state PADLOC results (t = 25 min)
Negative coolant flows in Branches 2, 4, and 5 (θ=1, Δt=60 sec)

<table>
<thead>
<tr>
<th>BRANCH 1</th>
<th>BRANCH 1, NO SOURCES</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME: 1.500000x10^3 s, 2.500000x10^1 time steps, DELTA t: 6.000000x10^-1 s, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 0</td>
<td></td>
</tr>
<tr>
<td>HE MASS FLOW RATE: 2.000000x10^1 G/S</td>
<td></td>
</tr>
<tr>
<td>BRANCH GLOBAL POINTS: BEGIN 4, END 1</td>
<td></td>
</tr>
</tbody>
</table>

| DIST. NDE CM | FLORETE CM | BULK A/CCM | FLUX A/(SCM*S) | PLATE OUT C A/SCM | COOL PLTOUT A/(SCM*S) | CROSS SECTION CM | WALL TEMP TEMP PRESS VELOC COEFF |
|-------------|------------|-----------|---------------|-----------------|-------------------|-----------------|------------------|---------|
| 1 0.000 | 2.197x15 | 1.471x05 | 0.000 | 1.766x07 | 0.000 | 7.850x01 | 3.142x00 | 500.0 | 500.0 | 30.0 | 1.391x04 | 1.905x01 |
| 2 3.000000 | 2.197x15 | 1.471x05 | 0.000 | 1.766x07 | 0.000 | 7.850x01 | 3.142x00 | 500.0 | 500.0 | 30.0 | 1.391x04 | 1.905x01 |
| 3 1.000x01 | 2.197x15 | 1.471x05 | 0.000 | 1.766x07 | 0.000 | 7.850x01 | 3.142x00 | 500.0 | 500.0 | 30.0 | 1.391x04 | 1.905x01 |

<table>
<thead>
<tr>
<th>BRANCH 2</th>
<th>BRANCH 2, PLATEOUT REGION SOURCE: 2.2E7 ATOMS/(8*CM^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME: 1.500000x10^3 s, 2.500000x10^1 time steps, DELTA t: 6.000000x10^-1 s, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 0</td>
<td></td>
</tr>
<tr>
<td>HE MASS FLOW RATE: 1.200500x10^1 G/S</td>
<td></td>
</tr>
<tr>
<td>BRANCH GLOBAL POINTS: BEGIN 5, END 6</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>DIST. NDE CM</th>
<th>FLORETE CM</th>
<th>BULK A/CCM</th>
<th>FLUX A/(SCM*S)</th>
<th>PLATE OUT C A/SCM</th>
<th>COOL PLTOUT A/(SCM*S)</th>
<th>CROSS SECTION CM</th>
<th>WALL TEMP TEMP PRESS VELOC COEFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.000</td>
<td>3.623x15</td>
<td>1.066x05</td>
<td>2.200x07</td>
<td>4.294x07</td>
<td>0.000</td>
<td>2.200x07</td>
<td>3.142x00</td>
</tr>
<tr>
<td>2 3.000000</td>
<td>2.477x15</td>
<td>1.066x05</td>
<td>2.200x07</td>
<td>4.294x07</td>
<td>0.000</td>
<td>2.200x07</td>
<td>3.142x00</td>
</tr>
<tr>
<td>3 1.000x01</td>
<td>1.328x15</td>
<td>1.066x05</td>
<td>2.200x07</td>
<td>4.294x07</td>
<td>0.000</td>
<td>2.200x07</td>
<td>3.142x00</td>
</tr>
<tr>
<td>NODE</td>
<td>ATOM</td>
<td>BULK FLOW</td>
<td>PLATE</td>
<td>COOL PLANT</td>
<td>PLANT OUT</td>
<td>SECT.</td>
<td>PERIM TEMP</td>
</tr>
<tr>
<td>------</td>
<td>------</td>
<td>------------</td>
<td>-------</td>
<td>------------</td>
<td>-----------</td>
<td>-------</td>
<td>-------------</td>
</tr>
<tr>
<td>1</td>
<td>0.000</td>
<td>1.092*15</td>
<td>1.211+05</td>
<td>1.584+00</td>
<td>1.160+07</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>2.500+00</td>
<td>1.092*15</td>
<td>1.211+05</td>
<td>1.584+00</td>
<td>1.160+07</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3</td>
<td>1.000+00</td>
<td>1.092*15</td>
<td>1.211+05</td>
<td>1.584+00</td>
<td>1.160+07</td>
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| 10.000 | 1.000+15 | 3.675+04 | 1.683+01 | 3.519+06 | 0.000 | 0.000 | 2.827+01 | 1.885+01 | 500. | 500. | 30. | 1.574+02 | 1.069+00 |
| 2 0.000+00 | 1.000+15 | 3.675+04 | 1.683+01 | 3.519+06 | 0.000 | 0.000 | 2.827+01 | 1.885+01 | 500. | 500. | 30. | 1.574+02 | 1.069+00 |
| 3 1.000+01 | 1.000+15 | 3.675+04 | 1.201+01 | 3.519+06 | 0.000 | 0.000 | 2.827+01 | 1.885+01 | 500. | 500. | 30. | 1.574+02 | 1.069+00 |

| 2.500000+02 | 1.068+00 | 5.616+02 | 1.069+00 |
| 3.843+01 | 2.199+01 | 750. | 750. | 30. | 5.616+02 | 1.069+00 |

| 30. | 3.843+01 | 2.199+01 | 750. | 750. | 30. | 5.616+02 | 1.069+00 |

| 108.00 | 108.00 |

| 3.843+01 | 2.199+01 | 750. | 750. | 30. | 5.616+02 | 1.069+00 | 108.00 | 108.00 |
Figure 14, Example 3

Steady-state PADLOC results (t = 40 min)
All coolant flows positive (θ=1, Δt = 60 sec)

---

| STEP | 4.000000E+01 |
---|---|

BRANCH 1, NO SOURCES.
TIMES 2.000000E+03 S, 4.000000E+01 TIME STEPS, DELTAT 6.000000E+01 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK 0
HE MASS FLOW RATE 2.000000E+01 G/S
BRANCH GLOBAL POINTS, BEGIN 4, END 1

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<td>1.160E+07</td>
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<td>0.000</td>
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BRANCH 2, PLATE OUT REGION SOURCE #2.2E7 ATOMS/(S\_CM**2)
TIMES 2.000000E+03 S, 4.000000E+01 TIME STEPS, DELTAT 6.000000E+01 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK 0
HE MASS FLOW RATE 4.200000E+01 G/S
BRANCH GLOBAL POINTS, BEGIN 5, END 6

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<th>HE-COOLANT</th>
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<td>VELOC</td>
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<td>7.728*00</td>
<td>1.548*00</td>
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| BRANCH | 4 | BRANCH | 4 | NO SOURCES | TIME | 2.400000*03 S | 4.000000*01 TIME STEPS, DELTAT | 6.000000*01 S | NUMBER OF ITERATIONS FOR THE TOTAL NETWORK | 0 | HE MASS FLOW RATE = 1,000000*01 G/S | BRANCH GLOBAL POINTS, BEGIN 6, END 3 |
|--------|---|--------|---|------------|------|----------------|----------------|------------------------------------------|---|----------------|----------------|
|        |   |        |   |            |      |                |                |                                          |   |                |                |
| DIST.  | CM | ATOM BULK FLUX | SOURCE RTE | CONDUIT | HE-COOLANT | WALL TEMP | TEMP | VELOC | COEFF |
|        |    | K | C TO P | OUT | COOL. | PLTOUT | SECT. | PERIM. | TEMP | PRESS | VELOC | COEFF |            |
|        |    | MOL/S | A/CCM | A/(SCM*S) | A/CCM | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) |
| 1.0000 | 1.328*15 | 1.720*05 | 0.000 | 1.024*06 | 0.000 | 0.000 | 1.257*01 | 1.257*01 | 750 | 750 | 40 | 5.215*02 | 1.099*00 |
| 2.5000 | 1.328*15 | 1.720*05 | 0.000 | 1.024*06 | 0.000 | 0.000 | 1.257*01 | 1.257*01 | 750 | 750 | 40 | 5.215*02 | 1.099*00 |
| 3.1000 | 1.328*15 | 1.720*05 | 0.000 | 1.024*06 | 0.000 | 0.000 | 1.257*01 | 1.257*01 | 750 | 750 | 40 | 5.215*02 | 1.099*00 |

| BRANCH | 5 | BRANCH | 5 | NO SOURCES | TIME | 2.400000*03 S | 4.000000*01 TIME STEPS, DELTAT | 6.000000*01 S | NUMBER OF ITERATIONS FOR THE TOTAL NETWORK | 0 | HE MASS FLOW RATE = 1,000000*01 G/S | BRANCH GLOBAL POINTS, BEGIN 3, END 5 |
|--------|---|--------|---|------------|------|----------------|----------------|------------------------------------------|---|----------------|----------------|
|        |   |        |   |            |      |                |                |                                          |   |                |                |
| DIST.  | CM | ATOM BULK FLUX | SOURCE RTE | CONDUIT | HE-COOLANT | WALL TEMP | TEMP | VELOC | COEFF |
|        |    | K | C TO P | OUT | COOL. | PLTOUT | SECT. | PERIM. | TEMP | PRESS | VELOC | COEFF |            |
|        |    | MOL/S | A/CCM | A/(SCM*S) | A/CCM | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) | A/(SCM*S) |
| 1.0000 | 1.328*15 | 1.720*05 | 0.000 | 1.024*06 | 0.000 | 0.000 | 1.257*01 | 1.257*01 | 750 | 750 | 40 | 5.215*02 | 1.099*00 |
### Table 1: HE Coolant Parameters

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<td>M,THNSF</td>
</tr>
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<td>9.620*06</td>
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<td>1.183*06</td>
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<td>9.620*06</td>
<td>0.000</td>
<td>1.183*06</td>
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</table>

**Branch 6**

**Branch 6 NO SOURCES/Boundary Condition at GL POINT 2 IS 1.0E-15 MOLES/S**

**Time** 2,400000*03 S 4,000000*01 TIME STEPS DELTAT 6,000000*01 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 0

**Branch Global Points, BEGIN 2, END 5**

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<th>BULK FLUX</th>
<th>PLATE</th>
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<th>**** CONDUIT ****</th>
<th>**** HE-COOLANT ****</th>
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</thead>
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<td>A/CCM</td>
<td>A/(SCM*S)</td>
<td>A/CCM</td>
<td>M,THNSF</td>
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<td>1.000*15</td>
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<td>1.000*00</td>
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**Branch 7**

**Branch 7 NO SOURCES**

**Time** 2,400000*03 S 4,000000*01 TIME STEPS DELTAT 6,000000*01 S, NUMBER OF ITERATIONS FOR THE TOTAL NETWORK: 0

**HE Mass Flow Rate 3,000000*01 G/S**

**Branch Global Points, BEGIN 6, END 4**

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<td>MOL/S</td>
<td>A/CCM</td>
<td>A/(SCM*S)</td>
<td>A/CCM</td>
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<td>7.640*05</td>
<td>0.000</td>
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</table>
decay constant \( \lambda = 10 \text{ l/sec} \)

coolant flow rates \( \dot{m}_1 = \dot{m}_2 = \pm 42.0855 \text{ g/sec} \)

coolant and wall temperatures \( T_1 = T_2 = 800 \text{°C} \)

coolant pressures \( P_1 = P_2 = 50 \text{ atm} \)

branch lengths \( L_1 = L_2 = 10 \text{ cm} \)

hydraulic diameters (circular cross section) \( d_1 = d_2 = 2 \text{ cm} \)

coolant source rates \( (\dot{q}_c)_1 = (\dot{q}_c)_2 = 0 \)

plateout source rates \( (\dot{q}_s)_1 = 0 \)
\( (\dot{q}_s)_2 = 2.2 \times 10^7 \text{ atoms/cm}^2 \text{ sec} \)

sorption behavior LS in both branches

convection forced in both branches

The sorption constants in the sorption equations (64) and (65), page 66, are again assumed to be

\[
\begin{align*}
\text{AVPOR} & = 3.88 \\
\text{BVPOR} & = 3.73 \times 10^{3} \text{°K} \\
S_s & = 10^{20} \text{ atoms/cm}^2 \text{ (saturation surface concentration).}
\end{align*}
\]

Hand Calculations

We now use the basic branch equations (98) through (102) (page 92) for the steady-state concentrations of a decaying fission product with linear sorption characteristics. For convenience these equations are repeated here.

\[
C(x) = C(0) e^{-\omega x} + \frac{\dot{q}_c}{\omega} \left(1 - e^{-\omega x}\right), \tag{103}
\]

\[
S(x) = \frac{\dot{q}_s + h[C(x)-\alpha]}{\lambda + h \beta}, \tag{104}
\]

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where

\[ Q' = \frac{1}{v} \left[ q_c + \frac{P}{A} h \left( \alpha + \beta \frac{q_s - h \alpha}{\lambda + h \beta} \right) \right], \quad (105) \]

\[ \omega = \frac{1}{v} \left[ \lambda + \frac{P}{A} h \left( 1 - \frac{h \beta}{\lambda + h \beta} \right) \right]. \quad (106) \]

The sorption parameters \( \alpha \) and \( \beta \) are the coefficients in the sorption relation

\[ B(S) = \alpha + \beta S. \]

Since the pressures and temperatures are the same in both branches, the coolant concentration is continuous throughout the loop. To set up the global equation system for the branch inlet conditions, we can thus use the concentrations instead of fission product flow rates. The global system for \( C_1(o) \) and \( C_2(o) \) is simply

\[ C_1(o) = C_2(L_2) \quad \text{branch 1} \]

\[ C_2(o) = C_1(L_1) \quad \text{branch 2}. \]

Substitution of \( C_1(L_1) \) and \( C_2(L_2) \) with Eq. (103) yields

\[ C_1(o) - e^{-\omega_1 L_2} C_2(o) = \chi_2 \]

\[ e^{-\omega_1 L_1} C_1(o) - C_2(o) = -\chi_1 \]

where

\[ \chi_i = \frac{Q'}{\omega_i} \left( 1 - e^{-\omega_i L_i} \right). \]

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The solution to this system is

\[
C_1(o) = \frac{e^{-\omega L_2} \chi_1 + \chi_2}{1 - e^{-(\omega_{1L_1} + \omega_{2L_2})}} , \\
C_2(o) = \frac{\chi_1 + e^{-\omega_{1L_1}} \chi_2}{1 - e^{-(\omega_{1L_1} + \omega_{2L_2})}} .
\]

With \(C_1(o)\) and \(C_2(o)\) so given, the \(x\)-dependence of the coolant and plate-out concentrations can now be obtained using Eqs.(103) through (106). The sorption parameters \(\alpha\) and \(\beta\) in these equations were computed according to the sorption relations Eqs.(64) and (65) on page 66. For the mass transfer coefficients \(h\) appropriate relations for forced convection in circular tubes (Appendix A, Eq. (A1)) were used. The results of the hand calculations are presented in Table 5 on the following page.* This table also gives the results for steady-state conditions with the coolant flow reversed in the loop. For comparison, results of the corresponding PADLOC run are shown in Figures 15 and 16 on pages 131 and 132. Figures 17 and 18 (page 133, 137) are PADLOC printouts for steady-state conditions for positive and negative coolant flow rates. Again, the results of the hand calculations and the steady-state PADLOC results are in exact agreement.

* The details are found in Ref. 4.
Table 5
Example 4
Steady-State Values for Coolant Concentration C and Plateout Concentration S

<table>
<thead>
<tr>
<th>Branch</th>
<th>Positive Coolant Flow</th>
<th>Negative Coolant Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C [atoms/cm³]</td>
<td>S [atoms/cm²]</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x₁ = 0 cm</td>
<td>1.139E+5</td>
<td>8.703E+4</td>
</tr>
<tr>
<td>x₁ = 5 cm</td>
<td>1.116E+5</td>
<td>8.524E+4</td>
</tr>
<tr>
<td>x₁ = 10 cm</td>
<td>1.093E+5</td>
<td>8.350E+4</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x₂ = 0 cm</td>
<td>1.093E+5</td>
<td>2.001E+6</td>
</tr>
<tr>
<td>x₂ = 5 cm</td>
<td>1.116E+5</td>
<td>2.003E+6</td>
</tr>
<tr>
<td>x₂ = 10 cm</td>
<td>1.139E+5</td>
<td>2.005E+6</td>
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</table>
Fig. 15. Example 4: Coolant flows and fission product concentrations versus time ($\eta = 1$, $\Delta t = 0.5$ sec)
Fig. 16. Example 4: Concentrations versus x 
\((4 = 1, \Delta t = 0.5 \text{ sec})\)
**Figure 17, Example 4**

Steady-State PADLOC Results ($t = 6.5$ sec) for Positive Coolant Flows ($\Delta t = 0.5$ sec)

---

**BRANCH 1, BRANCH 1, IN SOURCES**

**HE MASS FLOW RATE** = 4.2045 + 56 sec

**BRANCH GLOBAL POINTS** Begin... End 2

---

**HE-COOLANT**

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<th>TEMP</th>
<th>TEMP</th>
<th>PRESS</th>
<th>VELOC</th>
<th>M. THNSF</th>
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<td>800</td>
<td>800</td>
<td>50</td>
<td>6.095 + 03</td>
</tr>
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<td>6.095 + 03</td>
<td>8.763 + 00</td>
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<td>800.0</td>
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<td>11</td>
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<td>800.0</td>
<td>50.0</td>
<td>6.095+03</td>
</tr>
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</table>
Figure 18, Example 4

Steady-State PADLOC Results (t = 10 sec) for Negative Coolant Flows
(θ=1, Δt= 0.5 sec)

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<thead>
<tr>
<th>Step 2.000000+01</th>
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<tbody>
<tr>
<td><strong>BRANCH TOTAL</strong></td>
</tr>
<tr>
<td><strong>BRANCH GLOBAL POINTS</strong></td>
</tr>
<tr>
<td><strong>TIME</strong></td>
</tr>
<tr>
<td><strong>TIME STEP</strong></td>
</tr>
<tr>
<td><strong>NUMBER OF ITERATIONS FOR THE TOTAL NETWORK</strong></td>
</tr>
<tr>
<td><strong>HE MASS FLOW RATE</strong></td>
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</tbody>
</table>

<table>
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<td><strong>TIME STEP</strong></td>
</tr>
<tr>
<td><strong>NUMBER OF ITERATIONS FOR THE TOTAL NETWORK</strong></td>
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<tr>
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<th><strong>PLTUUT</strong></th>
<th><strong>BELI</strong></th>
<th><strong>PERIM TEMP</strong></th>
<th><strong>TEMP PRESS</strong></th>
<th><strong>VELUC</strong></th>
<th><strong>COEFF</strong></th>
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<td><strong>FLUX</strong></td>
<td><strong>PLATE</strong></td>
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<td><strong>HTE</strong></td>
<td><strong>CMSS</strong></td>
<td><strong>ALL</strong></td>
<td><strong>HE COOLANT</strong></td>
<td><strong>M ETHNSF</strong></td>
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<td><strong>NDE</strong></td>
<td><strong>CM</strong></td>
<td><strong>WDL/S</strong></td>
<td><strong>A/CM</strong></td>
<td><strong>A/(CM^2 * S)</strong></td>
<td><strong>A/CM</strong></td>
<td><strong>A/(CM^2 * S)</strong></td>
<td><strong>SEQ</strong></td>
<td><strong>CM</strong></td>
<td><strong>C</strong></td>
<td><strong>ATM</strong></td>
<td><strong>CM/S</strong></td>
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<th><strong>CUUL</strong></th>
<th><strong>PLTUUT</strong></th>
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<td><strong>A/CM</strong></td>
<td><strong>A/(CM^2 * S)</strong></td>
<td><strong>SEQ</strong></td>
<td><strong>CM</strong></td>
<td><strong>C</strong></td>
<td><strong>ATM</strong></td>
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</table>

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<th><strong>TIME STEP</strong></th>
<th><strong>NUMBER OF ITERATIONS FOR THE TOTAL NETWORK</strong></th>
<th><strong>HE MASS FLOW RATE</strong></th>
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<tr>
<td>2.000000+01</td>
<td>1.000000+01 S</td>
<td>1.000000+01 S</td>
<td>0</td>
<td>4.208555+01 G/s</td>
</tr>
<tr>
<td>DIST.</td>
<td>FLUX</td>
<td>PLATE</td>
<td>**** SOURCE RTL</td>
<td>**** CONDUIT *****</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>-------</td>
<td>-----------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>NDE CM</td>
<td>MOL/S</td>
<td>A/CM</td>
<td>A/(SCM+S)</td>
<td>A/SCM</td>
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<tr>
<td>1.000</td>
<td>0.000</td>
<td>3.522</td>
<td>1.194 + 5</td>
<td>-1.95 + 5</td>
</tr>
<tr>
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<td>3.522</td>
<td>1.194 + 5</td>
<td>-1.95 + 5</td>
</tr>
<tr>
<td>3.000</td>
<td>0.000</td>
<td>3.522</td>
<td>1.194 + 5</td>
<td>-1.95 + 5</td>
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<tr>
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<td>-1.95 + 5</td>
</tr>
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<td>0.000</td>
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<td>1.194 + 5</td>
<td>-1.95 + 5</td>
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<td>3.522</td>
<td>1.194 + 5</td>
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<td>3.522</td>
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<td>-1.95 + 5</td>
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<td>3.522</td>
<td>1.194 + 5</td>
<td>-1.95 + 5</td>
</tr>
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</table>
REFERENCES


APPENDIX A

MASS TRANSFER COEFFICIENTS

PADLOC employs built-in mass transfer correlations for both forced and free convection. The general forms of these relations (Ref. 5) are given below.

a. forced convection:

\[
h = \frac{D}{\chi} \left[ \alpha_1 + \alpha_2 \left( \frac{d}{L} \right)^{\alpha_3} \right] \frac{\alpha_4}{Re} \frac{\alpha_5}{Sc} \], \quad (A1)
\]

and

b. free convection:

\[
h = \frac{D}{\chi} \beta_1 Re^{\beta_2} \frac{\beta_3}{Sc} \frac{\beta_4}{Gr} \frac{d^{\beta_5}}{L} \]. \quad (A2)
\]

Here,

- \( h [\text{cm/sec}] \) = mass transfer coefficient
- \( D [\text{cm}^2/\text{sec}] \) = diffusion coefficient of fission product in helium
- \( Re \) = Reynolds Number
- \( Sc \) = Schmidt Number
- \( Gr \) = Grashof Number
- \( d [\text{cm}] \) = hydraulic diameter of conduit
- \( L [\text{cm}] \) = hydrodynamic entry length, and,
- \( \chi \equiv L \) for flat plates
- \( \chi \equiv d \) for other geometries.
The values for \( \alpha \) and \( \beta \) for the different flow regimes and geometries are given in Tables A1 and A2 on the following pages. These tables also show the values of the PADLOC input flow indicators KGF, KGN, KGNFP of card B8.

The definitions of the dimensionless flow parameters are as follows:

1. \[ \text{Re} = \frac{v p d}{\mu}, \]  
   where 
   \[ v [\text{cm/sec}] = \text{average coolant velocity}, \]
   \[ \rho [g/cm^3] = \text{helium density}, \]
   \[ \mu [g/(cm-sec)] = \text{dynamic viscosity of helium}, \]
   \[ d [cm] = 4 A/P, (A = \text{cross section area,} P = \text{wetted perimeter}). \]

2. \[ \text{Sc} = \frac{\mu}{\rho D}. \]  

3. \[ \text{Gr} = g L^3 \left| \rho_m - (\rho_m)_\infty \right| \frac{\rho_m}{2} \frac{\mu_m}{\rho_m}. \]

In Eq. (A5) the index \( m \) stands for mixture of fission product and helium coolant, \( (\rho_m)_\infty \) is the average density in the free stream, \( g \) is the acceleration of gravity. The formula for the diffusion coefficients (Ref. 5) is

\[ D \text{[cm}^2 / \text{sec]} = 0.1682 \left( \frac{T_c}{1000} \right)^{1.65} \left( \frac{23.83}{p[\text{atm}]} \right) \sqrt{\frac{1}{M[g/mol]} + 0.257}, \]  

2-A
**Table A1**

**KGF and a Values for Forced Convection**

<table>
<thead>
<tr>
<th>Geometry</th>
<th>KGF</th>
<th>Flow Regime</th>
<th>(a_1)</th>
<th>(a_2)</th>
<th>(a_3)</th>
<th>(a_4)</th>
<th>(a_5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow in tube and annular flow</td>
<td>1</td>
<td>(\text{Re}&lt;2100) (laminar) (\frac{L}{d \text{Re} \text{Sc}} \geq 0.07)</td>
<td>0</td>
<td>3.66</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\frac{L}{d \text{Re} \text{Sc}} &lt; 0.07)</td>
<td>0</td>
<td>1.86</td>
<td>0.33</td>
<td>0.33</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{Re}\geq2100) (turbulent)</td>
<td>0</td>
<td>0.023</td>
<td>0</td>
<td>0.8</td>
<td>0.33</td>
</tr>
<tr>
<td>Aligned tube bundles in cross flow (use (d) = outer tube diameter)</td>
<td>2</td>
<td>(\text{Re}_{\text{max}} &lt;1000)</td>
<td>(f(\text{Re};0.43,0,10^3))</td>
<td>(f(\text{Re};0.52,0.27,10^3))</td>
<td>0</td>
<td>(f(\text{Re};0.5,0.63,10^3))</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1000 \leq (\text{Re})_{\text{max}} &lt; 200000)</td>
<td>0</td>
<td>0.27</td>
<td>0</td>
<td>0.63</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((\text{Re})_{\text{max}} \geq 200000)</td>
<td>0</td>
<td>0.02</td>
<td>0</td>
<td>0.84</td>
<td>0.36</td>
</tr>
<tr>
<td>Staggered tube bundles in cross flow (use (d) = outer tube diameter)</td>
<td>3</td>
<td>((\text{Re})_{\text{max}} &lt;1000)</td>
<td>(f(\text{Re};0.43,0,10^3))</td>
<td>(f(\text{Re};0.60,0.40,10^3))</td>
<td>0</td>
<td>(f(\text{Re};0.5,0.60,10^3))</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1000 \leq (\text{Re})_{\text{max}} &lt; 200000)</td>
<td>0</td>
<td>0.40</td>
<td>0</td>
<td>0.60</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((\text{Re})_{\text{max}} \geq 200000)</td>
<td>0</td>
<td>0.021</td>
<td>0</td>
<td>0.84</td>
<td>0.36</td>
</tr>
<tr>
<td>Flat plate (use plate length for Reynold's number evaluation)</td>
<td>4</td>
<td>(\text{Re}&lt;3.2\times10^5) (laminar) (0 \leq \text{Sc} \leq 0.6)</td>
<td>0</td>
<td>0</td>
<td>(f(\text{Sc};1.128,0.664,0.6))</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0.6 &lt; \text{Sc} \leq 10)</td>
<td>0</td>
<td>0.664</td>
<td>0</td>
<td>0.5</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{Sc} &gt; 10)</td>
<td>0</td>
<td>0.678</td>
<td>0</td>
<td>0.5</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\text{Re}\geq3.2\times10^5) (turbulent)</td>
<td>0</td>
<td>0.037</td>
<td>0</td>
<td>0.8</td>
<td>0.33</td>
</tr>
</tbody>
</table>

\[ f(x; a, b, c) = a - \left(\frac{(a-b)(2c-x)x}{c^2}\right) \]
Table A2
KGN and $\delta$ Values for Free Convection

<table>
<thead>
<tr>
<th>Geometry</th>
<th>KGN</th>
<th>Flow Regime</th>
<th>$\beta_1$</th>
<th>$\beta_2$</th>
<th>$\beta_3$</th>
<th>$\beta_4$</th>
<th>$\beta_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow in tube and annular flow</td>
<td>1</td>
<td>Re $Sc \ d/L \leq 30$</td>
<td>6</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Re $Sc \ d/L &gt; 30$</td>
<td>1.78</td>
<td>0.357</td>
<td>0.357</td>
<td>0</td>
<td>0.357</td>
</tr>
<tr>
<td>Vertical tube banks and vertical flat plates</td>
<td>2</td>
<td>$Gr \ Sc &lt; 10^4$</td>
<td>1.295</td>
<td>0</td>
<td>0.1646</td>
<td>0.1646</td>
<td>0</td>
</tr>
<tr>
<td>(KGNFP=1)</td>
<td></td>
<td>$10^4 &lt; Gr \ Sc &lt; 10^9$</td>
<td>0.59</td>
<td>0</td>
<td>0.25</td>
<td>0.25</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$Gr \ Sc \geq 10^9$</td>
<td>0.33</td>
<td>0</td>
<td>0.13</td>
<td>0.33</td>
<td>0</td>
</tr>
<tr>
<td>Horizontal tube banks and horizontal flat</td>
<td>3</td>
<td>$Gr \ Sc &lt; 10^{-5}$</td>
<td>0.4</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>plates (KGNFP=1)</td>
<td></td>
<td>$10^{-5} &lt; Gr \ Sc &lt; 10^4$</td>
<td>1.962</td>
<td>0</td>
<td>0.1381</td>
<td>0.1381</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$10^4 &lt; Gr \ Sc &lt; 10^9$</td>
<td>0.53</td>
<td>0</td>
<td>0.25</td>
<td>0.25</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$Gr \ Sc \geq 10^9$</td>
<td>0.13</td>
<td>0</td>
<td>0.33</td>
<td>0.33</td>
<td>0</td>
</tr>
</tbody>
</table>
where $M$ is the molecular mass of the fission product species, and the dynamic viscosity is computed (from Ref. 6) as

$$\mu \left[ \frac{g}{cm \cdot sec} \right] = 5.31 \times 10^{-5} \left( \frac{T_c (°K)}{1273} \right)^{0.678}.$$  \hspace{1cm} (A7)

Relevant PADLOC input consists of

- $m [g/sec] = $ helium mass flow rate,
- $p [atm] = $ helium pressure,
- $T_c (°C) = $ helium temperature, and,
- $T_w (°C) = $ wall temperature.

With this input, the density is calculated from the perfect gas law,

$$\rho = \frac{M_p}{RT},$$ \hspace{1cm} (A8)

where $R = 82.057$ atm. cm$^3$/(g mole °K) is the universal gas constant. The coolant velocity follows from

$$v = \frac{m}{\rho A} = \frac{R}{M} \frac{T}{A p}.$$ \hspace{1cm} (A9)