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ICEDF: A Code for Aerosol Particle Capture in Ice Compartments

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ABSTRACT

This report describes the technical bases and use of the computer code ICEDF. ICEDF was developed to estimate the extent of particle retention in the ice compartments of pressurized water reactor (PWR) ice condenser containment systems during severe accidents. This report also serves as a complete user's guide for the most recent stand-alone version of ICEDF. A complete code description, code operating instructions, code listing, examples of the use of ICEDF, and a summary of a parameter sensitivity study support the use of code ICEDF.

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EXECUTIVE SUMMARY

This report describes the technical bases and use of the computer code ICEDF. The code was developed to estimate particle retention in the ice compartments of pressurized water reactor (PWR) ice condenser containment systems during severe accidents. ICEDF and other codes are products of a broader U.S. Nuclear Regulatory Commission (NRC) study of the particle retention effectiveness of Engineered Safety Features (ESFs). Pacific Northwest Laboratory (PNL) is conducting the study for the NRC.

The technical bases of code ICEDF consist of the particle removal mechanisms presented in an earlier PNL report, NUREG/CR-3248, and particle growth calculation methods recently developed at PNL. The particle removal mechanisms modeled in ICEDF are gravitational settling, impaction and interception, Brownian diffusion, diffusiophoresis, and thermophoresis. The particle growth methods use the principles of cloud physics and heat and mass transfer and are important in enhancing settling, impaction, and interception removal mechanisms.

This report is also intended to serve as a complete ICEDF user's manual. In this function the following items are included: 1) ICEDF code description with methods/algorithms of calculation and subroutines; 2) code operating instructions with input requirements, output descriptions, parameter selection guidelines, and examples of ICEDF use; 3) a parameter sensitivity study summary; and 4) a complete list of ICEDF with subroutines.

A brief description of experiments planned for use in future validation efforts is also presented.

1.0 INTRODUCTION

The ice condenser system for containment pressure suppression is one of many types of Engineered Safety Features (ESFs) installed in U.S. commercial nuclear power reactors to control and mitigate the consequences of occurrences that might challenge reactor integrity and/or adversely affect plant personnel or the public. This report is the result of a study funded by the U.S. Nuclear Regulatory Commission (NRC) at Pacific Northwest Laboratory (PNL) to assess the fission product retention effectiveness of ESF systems under hypothetical severe accident conditions.

Although the ice condenser system is designed to condense steam in the containment building of certain pressurized water reactors (PWRs), the primary objective of the ESF study is to assess the particle removal capability of the ice condenser design. A predecessor PNL report, NUREG/CR-3248 (Winegardner et al. 1983), provides most of the technical background for the computer code ICEDF. The objective of developing ICEDF was to provide a method for predicting ice compartment particle retention during postulated severe accidents where conditions change rapidly, making hand calculations impractical. An early version of ICEDF was modified and adapted to a containment aerosol code for recent severe accident source term analyses (Gieseke et al. 1984).

This report discusses the most recent stand-alone version of ICEDF. Chapter 2 reviews the technical bases of this code, which includes the particle capture mechanisms discussed in NUREG/CR-3248 (Winegardner et al. 1983) and recently developed particle growth mechanisms. Chapter 3 discusses code organization, methods and algorithms of the calculations, and subroutines. Chapter 4 provides the details for using the code including input requirements, output description, parameter selection guidelines, and examples of ICEDF use. Chapter 5 discusses the status of ICEDF validation. Appendix A summarizes a parameter sensitivity study, and Appendix B is a recent code list.

2.0 TECHNICAL BASES SUMMARY

The version of the ICEDF code described in this report was developed in two separate phases. The initial version was based almost solely on the equations for particle capture that were developed by Winegardner, Postma, and Jankowski, and presented in NUREG/CR-3248, Studies of Fission Product Scrubbing Within Ice Compartments. These retention equations are reproduced in Section 2.1 of this report. Although neglected in the initial effort, NUREG/CR-3248 also noted that the potential for enhanced removal upon particle growth by water vapor pickup should be investigated as part of the effort to attain the goal of making realistic estimates of particle retention. As a result, analytical models to calculate the extent of growth in the presence of condensible vapors were subsequently developed and incorporated into the code. The resulting equations, including those for the growth of soluble nuclei in unsaturated conditions as well as those for condensational growth arising from a supersaturated vapor (from the mixing of the hot, moist gas from an accident with the cool gas already in the ice compartment) are developed in Section 2.1.

2.1 SUMMARY OF PARTICLE CAPTURE MECHANISMS IN NUREG/CR-3248

The particle capture mechanisms considered in NUREG/CR-3248 were gravity settling, impaction and interception, Brownian diffusion, diffusiophoresis, thermophoresis, and turbulent deposition. Because turbulent deposition is considered negligible for most of the velocities predicted in the ice bed, the model developed for this latter mechanism was not incorporated into the code.

To illustrate the ICEDF mechanisms quantitatively, consider a particle mass balance over a control volume of gas flowing vertically between ice baskets. This volume or node is considered to be at steady state and well mixed; i.e., the particle concentration of the gas within the node is the same as that of the gas leaving the node. The mass balance can then be written as

$$G_i C_{gi} = K_s C_{go} + K_I C_{go} + K_{BD} C_{go} + K_D C_{go} + K_T C_{go} + G_o C_{go} , \qquad (2.1)$$

where

G = gas flow rate, m^3/s

C = airborne concentration, g/m^3

K = removal rate constant, m^3/s.

The subscripts have the following meaning:

i = conditions at node inlet

g = in the gas phase

s = settling

I = impaction and interception

BD = Brownian diffusion

D = diffusiophoresis

T = thermophoresis

o = conditions at node outlet.

The ratio of the inlet to the outlet particle rate (G_iC_{gi}/G_oC_{go}) is defined as the decontamination factor (DF). Rearrangement of Equation 2.1 in terms of this ratio results in the following expression for the DF of the well-mixed node.

$$DF = 1 + \sum_i K_i/G_o \ . \tag{2.2}$$

The overall column DF for n nodes in series is then given by

$$DF = DF(1)DF(2)\ .\ .\ .\ DF(n)\ . \tag{2.3}$$

Finally, it is necessary to consider the nodal DF for each particle size j, DF_j, in the gas stream. Hence,

$$DF_j = 1 + \sum_i K_{ij}/G_o \ , \tag{2.4}$$

where K_{ij} is the removal rate constant for particle size 'j' by mechanism 'i'. The remainder of Section 2.1 lists the equations used to describe the various rate constants.

2.1.1 Gravity Settling

The expression for the rate constant associated with gravity settling, K_{sj}, is the product $V_{sj}A_s$, where V_{sj} is the particle settling velocity, cm/s and A_s is the available horizontal upward facing surface area, cm^2.

For particles having aerodynamic equivalent diameters (AED) <70 μm, V_{sj} normally follows Stokes law for spherical particles:

$$V_{sj} = \rho_j d_j^2 \; g \; Cn_j / 18 \, \mu \; , \qquad (2.5)$$

where

ρ_j = effective particle density, g/cm^3

d_j = effective particle diameter, cm

g = acceleration of gravity, 980 cm^2/s

Cn_j = Cunningham correction factor (see subroutine DIFFU, Section 3.3)

μ = bulk gas viscosity, poise.

For particles of d_j >70 μm, ICEDF uses a series of empirical expressions to find V_{sj} (see subroutine VSET, Section 3.3.4). The area A_s is an important parameter; its selection is discussed in Section 4.1.1.

2.1.2 Impaction and Interception

The ice baskets and support structures have a large number of surfaces that can serve as targets for removal by impaction and interception. The impaction/interception removal rate constant is

$$K_I = V_I \; A_I \; \varepsilon_I \; , \qquad (2.6)$$

where

V_I = gas velocity approaching the segment, cm/s

A_I = projected area perpendicular to the flow, cm^3

ε_I = impaction/interception efficiency.

The efficiency is

$$\varepsilon_I = \frac{Stk^2}{(Stk + 0.05)^2} - 0.04 + 2\frac{d_j}{d_c} , \qquad (2.7)$$

where Stk is the Stokes number ($V_I \rho_j d_j^2\ Cn_j/9\mu d_c$) and d_c is the collector diameter, cm.

2.1.3 Brownian Diffusion

For particles <0.1 μm diameter, Brownian diffusion becomes important as a capture mechanism. The Brownian removal rate constant is defined as

$$K_{BDj} = V_I\ A_{BD}\ \varepsilon_{BDj} , \qquad (2.8)$$

for flow perpendicular to capture surfaces. Here

V_I = gas velocity approaching the surface, cm/s

A_{BD} = projected area for diffusional deposition, cm^2

ε_{BDj} = diffusional capture efficiency.

The efficiency ε_{BDj} for cylinders is

$$\varepsilon_{BDj} = \frac{1}{Pe_j} + 1.727\ Re^{1/6}/Pe_j^{2/3} , \qquad (2.9)$$

where

Pe_j = Peclet number = $d_c V_I/D_j$

Re = Reynolds number = $\rho D_c V_I/\mu$

D_j = particle diffusivity, cm^2/s, = $kTCn_j/3\pi\mu d_j$ (Stokes-Einstein equation)

T = absolute temperature, °K

k = Boltzmann constant.

For flow parallel to the capture surface, the removal rate constant K_{BDj} is related to particle mass transfer coefficients by the relationship

$$K_{BDj} = \sum_{l} K_{jl} A_{l}, \tag{2.10}$$

where

K_{jl} = mass transfer coefficient for the j-th particle size to the l-th surface, cm/s,

A_{l} = surface area of the l-th surface, cm^2.

Correlations are available for the mass transfer coefficients. For natural convection in ice beds

$$\frac{K_j}{D_j} = 0.13\ (Gr\ Sc_j)^{1/3}/\ell\ , \tag{2.11}$$

where

K_j = j-th particle size mass transfer coefficient, cm/s

Gr = Grashof number = $(\rho z^3 g/\mu^2)\Delta\rho$

Sc_j = Schmidt number = $\mu/\rho D_j$

ρ = bulk gas density, g/cm^3

$\Delta\rho$ = density difference between bulk gas and gas at the surface, g/cm^3

ℓ = characteristic length of surface in direction of flow, cm.

Equation (2.11) is preferred over forced convection correlations in ICEDF, since the flow rates along the ice are likely to be strongly influenced by density instabilities. For forced convection flow, other types of correlations for the Sherwood number, $K_j\delta/D_j$, can be used. Here, δ is some characteristic dimension of the flow system (e.g., the hydraulic radius of the flow path between ice baskets).

2.1.4 Diffusiophoresis

The deposition velocity used to develop the removal rate constant for diffusiophoresis, K_D, is based on consideration of both Stefan flow and the molecular weight gradient arising from steam condensation. For steam air mixtures these two mechanisms are opposing with Stefan flow dominating. Consideration of the above results in the following equation for the rate constant, an expression that is independent of particle size.

$$K_D = 0.9G_o\left(\frac{X_{2o}X_i}{X_{2i}} - X_o\right), \tag{2.12}$$

where

G_o = volume flow rate of gas at outlet of node

X_{2o} = node outlet mole fraction of air

X_i = node inlet mole fraction of steam

X_{2i} = node inlet mole fraction of air

X_o = node outlet mole fraction of steam.

2.1.5 Thermophoresis

The following equation, an expression to predict the extent of removal resulting from the fact that the capture target can be colder than the gas, was developed for the thermophoretic deposition rate constant K_{Tj}.

$$K_{Tj} = G_o\ C_{Tj}\ (T_i - T_o)/\alpha\ , \tag{2.13}$$

where

C_{Tj} = constant defined below

T_i = node inlet temperature, °K

T_o = node outlet temperature, °K

α = gas thermal diffusivity, cm^2/s.

The constant C_{Tj} depends on the diameter of particle j (Davies 1966):

$$C_{Tj} = \frac{3\mu}{2\rho T}\,Cn_j[k_g/k_p + C_t\ Kn_j]/[(1 + 3\ C_m\ Kn_j)(1 + 2\ kg/kp + 2\ C_tKn_j)], \tag{2.14}$$

where

k_g/k_p = ratio of thermal conductivities of gas/particle

C_t = thermal accommodation constant

Kn_j = Knudsen number = $\frac{\text{gas mean free path}}{\text{j-th particle radius}}$

C_m = momentum accommodation constant.

2.1.6 Overall Decontamination Factors

In ICEDF the expressions for diffusiophoretic and thermophoretic DF are considered as separate factors in the overall expression for nodal DFs of each particle size. Thus for the k-th node and j-th particle size

$$DF_j(k) = \left(1 + \frac{K_{Dj}}{G_o}\right)_k \left(1 + \frac{K_{Tj}}{G_o}\right)_k \left[1 + (K_{sj} + K_{BDj} + K_{Ij})/G_o\right]_k . \quad (2.15)$$

Then for the series of n nodes [Equation (2.3)]

$$DF_j = \prod_{k=1}^{n} DF_j(k) , \quad (2.16)$$

and to obtain an overall DF for all particles over all nodes

$$DF = \sum_j \dot{m}_j / \sum_j \dot{m}_j/DF_j , \quad (2.17)$$

where

$\dot{m}_j$ = inlet mass flow rate of particle size j, g/s.

Equations (2.15), (2.16), and (2.17) comprise the core of calculations in ICEDF. All other computations serve to support the calculations of the various removal rate constants and to interpret the output data.

2.2 PARTICLE GROWTH

As indicated earlier, particle growth was neglected in the development of the initial version of the ICEDF code, a version that was based almost entirely on the above capture equations. Because of the possible significant enhancement effect, most of the work that has been conducted since the development of the initial model has focused on the growth of aerosol particles by condensation. The technical bases for condensational growth models for both unsaturated and supersaturated environments is discussed below. Before proceeding, note that it is assumed that agglomeration effects can be neglected because of aging.

2.2.1 Growth in Supersaturated Atmospheres

A supersaturated atmosphere exists in many cases when rapid cooling of near-saturated gas occurs. To discuss this phenomena quantitatively, the degree of saturation, S, is defined as

$$S = P_v / P_v^o , \tag{2.18}$$

where P_v is the actual partial pressure of water vapor in the gas, and P_v^o is the equilibrium water vapor pressure at the pressure and temperature of the gas for a plane surface. For $S < 1$, the gas is subsaturated. When $1 < S < 4$, supersaturated vapors can condense on heterogeneous wettable surfaces. When $S > 4$, water vapor can condense by homogeneous droplet nucleation and growth as well as on heterogeneous surfaces (Pruppacher and Klett 1980).

The rate of heterogeneous particle growth is of primary concern when considering ice bed depletion of particles from the gas phase. In the flow regime of the ice bed, two processes limit the growth rate. The first process is the rate of sensible heat loss from the gas to the ice relative to the rate of latent heat loss that condenses vapors on the ice. The second process is the condensation rate on individual particles. This latter rate limiting step is considered next.

The classical rate equation, called Mason's equation, for growth of droplets in rain clouds is found in the fundamental theories of cloud physics; it is derived in Byers (1965) as

$$r\frac{dr}{dt} = (S-S')/[(M_{wv} \Delta H_v^2 \rho_L / kgRT^2) + (\rho_L RT/P_v^o DM_{wv})] , \tag{2.19}$$

where

r = droplet radius, cm

t = time

M_{wv} = molecular weight of the vapor, 18 g/g-mole

ΔH_v = latent heat of vaporization, j/g

ρ_L = density of condensed liquid, g/cm^3

kg = gas thermal conductivity, j/cm s

R = gas constant

T = absolute temperature, °K

D = vapor diffusivity in gas, cm^2/s

S' = actual saturation level at droplet surface(a).

Equation (2.19) is more simply written as

$$r\frac{dr}{dt} = \frac{S-S'}{a+b} \qquad (2.20)$$

and is used in its integrated form (for constant, S, a, and b) as

$$r^2 = r_o^2 + \frac{2\,(S-S')}{a+b}\,(t - t_o)\ . \qquad (2.21)$$

Mason's equation accounts for both the diffusive resistance of the condensing vapor as well as the conductive resistance of the gas surrounding the droplet that inhibits the removal of the latent heat of condensation. The above equations are used in ICEDF along with empirical relationships for the constants a(T) and b(T).

The remaining growth-limiting process, related to heat removal, requires detailed mass and energy balances to be described quantitatively. First, recall that the calculational node is a well-mixed control volume. At steady state, the mass balances rate equations can be written as

$$\dot{M}(NC)_i = \dot{M}(NC)_o\ , \qquad (2.22)$$

(a) The Kelvin equation relates the droplet diameter d_o' to the droplet saturation level (Adamson 1976):

$$d_o' = 4\sigma\,\tilde{V}/RT\,\ln(S')$$

where $\tilde{V}$ is the liquid molar volume, cm^3/g mole.

$\dot{M}(NC)_i$ and $\dot{M}(NC)_o$ are the noncondensible mass flow rates at inlet and outlet, respectively.

For j-size particles (P_j)

$$\dot{M}(P_j)_i = \dot{M}(P_j)_o + \dot{M}(P_j)_i\ (1 - 1/DF_j). \qquad (2.23)$$

For water

$$\dot{M}(w)_i = \dot{M}(wv)_i + \dot{M}(cw)_i \qquad (2.24a)$$

$$\dot{M}(cw)_i = \sum_j \dot{M}_j(cw)_j \qquad (2.24b)$$

$$\dot{M}(cw)_i = \dot{M}(wv)_o + \dot{M}(cw)_o + \dot{M}(w\ell)\ , \qquad (2.24c)$$

where

$\dot{M}_j(cw)_i$ = mass rate of condensed water on j-sized particles, g/s

w = water

v = water vapor

cw = condensed water.

The water loss rate $\dot{M}\ (w\ell)$ is

$$\dot{M}(w\ell) = p\Delta z h_c(T_i - T_w)/\Delta H_v + \sum_j \dot{M}_j(cw)_i\ (1 - 1/DF_j)\ , \qquad (2.25)$$

where

p = ice perimeter of flow channel, cm

h_c = condensational heat transfer coefficient, watts/cm^2°K

T_w = water film wall temperature, °K

Δz = thickness of control volume in flow direction, cm.

The energy balance across the node is similar. Define the enthalpy flow rate of the aerosol as $\dot{E}$, then

$$\dot{E}_i = \dot{E}_o + \dot{Q} \ , \tag{2.26}$$

where $\dot{Q}$, watts, is the energy loss rate to the ice in the thickness Δz. A more detailed definition of $\dot{Q}$ is given by

$$\dot{Q} = p\Delta z\left[(h_c + h_s)^{-1} + \frac{\Delta x}{k_w}\right]^{-1} (T_i - T_w) \\ + \sum_j \dot{M}_j (cw)_i \ (1 - 1/DF_j) \left[Cp_w + (1 - fw_{ij})\ Cp_s/fw_{ij}\right](T_i - T') \ , \tag{2.27}$$

where

1st term on rhs = condensation and sensible heat loss rates

2nd term on rhs = enthalpy loss because of particle capture

h_s = sensible heat transfer coefficient, watts/cm^2°K

Cp_w = condensed water heat capacity, J/g°K

k_w = water film thermal conductivity, watts/cm°K

Δx = water film thickness, cm

Cp_s = solid particle heat capacity, J/g°K

fw_{ij} = weight fraction of water in inlet for j-th particle size

T' = enthalpy reference temperature (273.2°K here).[a]

To complete the details of the energy balance, the expression for $\dot{E}_i$ is

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[a] In Equations (2.25) and (2.27), the inlet temperature T_i is used instead of T_o, the outlet or well-mixed volume temperature. This simplifies calculations and introduces minimal error for small Δz.

$$\dot{E}_i = \{\dot{M}(NC)_i \, Cp_{NC} + \sum_j [\dot{M}_j(cw)_i \, Cp_w + (1 - fw_{ij})Cp_s/fw_{ij}]$$

$$+ \dot{M}(wv)_i \, Cp_v\} \, (T_i - T') + \dot{M}(wv)_i \, \Delta H_v \; , \qquad (2.28)$$

where

Cp_v = water vapor heat capacity, J/g°K.

A similar expression can be written for $\dot{E}_0$. The solution of the above equation for the outlet values neglecting condensation on droplets is discussed in more detail in Chapter 3.0. A last necessary step is needed for adjusting the outlet quantities if $S_0(T_0) > 1$ to allow for condensation for the thermodynamic limit in particle growth. This requires that the outlet gas be at $S_0(T'_0) = 1$. This new (higher) temperature T'_0 is obtained from $\dot{E}_0$ with a net loss in $\dot{M}(wv)_0$ and gain in $\dot{M}(cw)_0$. The algorithms for this adjustment are also discussed in Chapter 3.0.

Note that a more rigorous method of solution for particle growth was considered. This method involved a simultaneous solution of the complete set of first-order derivations of all variables along the flow path. The method would have required a completely new beginning for ICEDF, which already had a nodalized system without particle growth. Another disadvantage of the more rigorous method was the high degree of 'stiffness' of the set of equations. For these two reasons, the rigorous method was dropped, and the ICEDF code evolved into the calculational system to be described in Chapter 3.0.

2.2.2 Soluble Particle Growth

Although not separated in reality, soluble particle growth is considered independent of the growth induced by supersaturation. The two growth phenomena are treated separately to facilitate calculations. Specifically it is assumed that soluble substances in the particles are dissolved in water and are in equilibrium with the subsaturated ($S < 1.0$) atmosphere. Growth is frozen at $S = 0.99$ because of this phenomenon. When $S > 1.0$, growth proceeds according to the equations presented in Section 2.2.1, but with the initial diameter equal to the equilibrium particle diameter at $S = 0.99$. The cutoff at $S = 0.99$ is based on technical judgment. Experimental comparison of growth phenomena with soluble and insoluble particles are needed to better define the value.

The equilibrium drop size reached in a humid atmosphere is governed by the degree to which the vapor pressure of water is lowered by the soluble material and the degree to which curvature affects an increase in the vapor pressure. Both effects are well understood and are calculable using classical physics and chemistry. The equilibrium saturation ratio, S, is related to drop size by an equation presented by Fletcher (1962).

$$S = \frac{\exp\left(\frac{2\sigma}{n_L kTr}\right)}{1 + \left[\frac{imMw_o}{Mw(\frac{4}{3}\pi r^3 \rho - m)}\right]} \qquad (2.29)$$

where

S = saturation ratio (the relative humidity)

σ = surface tension of solution, dyne/cm

n_L = number of molecules/cm^3 of solution (solvent + solute)

r = radius of drop, cm

i = van't Hoff ionization factor

ρ = density of solution, g/cm^3

Mw = molecular weight of solute, g/g mole

Mw_o = molecular weight of solvent, g/g mole

m = mass of solute in the droplet, g.

Equation (2.29) was evaluated under the assumption that the solute was cesium hydroxide, the solvent water, and the temperature 100°C. Results are summarized in Table 2.1.

The data of Table 2.1 illustrate that particle growth factors depend on relative humidity, S, and that significant growth factors are predicted.

TABLE 2.1. Growth of CsOH Particles in Humid Atmosphere at 100°C

Dry Particle Radius, μm	Droplet Radius in Stated Humidity			
	S = 0.9	S = 0.95	S = 0.99	S = 0.999
0.01	0.0195	0.0225	0.0295	0.0345
0.10	0.195	0.255	0.425	0.775
1.0	1.95	2.55	4.45	9.35
10.0	19.5	25.5	44.5	95.5

3.0 ICEDF CODE DESCRIPTION

This chapter provides details of the ICEDF code organization, the calculation methods/algorithms, and subroutines used. The code began as a simple combination of the DF calculations of NUREG/CR-2348 and evolved into a more complex system incorporating mass and energy balances for the gas phase along with particle-growth calculations in supersaturated atmospheres.

3.1 CODE ORGANIZATION

The ICEDF code does not follow the recent trends of 'structured' programming, where the main code is essentially a driver of many subroutines. The main code in ICEDF is centered around DF calculations for a series of nodes corresponding to the gas flow path in the ice bed. It is supported by calculations of removal rate constants, particle-size changes, heat and mass balances, and thermodynamic conditions. There are seven subroutines involved in the supporting calculations. Figure 1 represents a flow chart of the main program of ICEDF. A brief discussion of each block in the flow chart follows.

3.1.1 Read/Write Input

The input data are read in and reprinted immediately using a free-field format. The input data consist of ice bed physical parameters and inlet aerosol characteristics throughout the accident sequence.

3.1.2 Define Fixed Variables

A number of constants used in various equations are defined. An important vector, DPART(J), is defined in a DATA statement. DPART(J) represents the particle sizes as equivalent spherical diameters (in centimeters) in J = 1, ... 20 buckets. This vector can be changed by the user by recompiling the program. The existing DATA DPART/statement provides a set of 20 sizes representing a lognormal distribution about 1 μm (10^{-4} cm) for the inlet aerosol if the input file particle concentrations are a constant multiple of the example file (cf., Section 4.1).

3.1.3 Output DO Loop

The user has specified the number (KOUT) of output times that DF calculations are to be made. At a corresponding set of times, TOUT (K = 1, ... KOUT), the ICEDF code interpolates all changing input conditions to correspond to each TOUT(K) and follows a volume of aerosol from the inlet of the ice bed to the outlet.

3.1.4 Input Massage

First the code takes the appropriate TOUT(K) value to interpolate between time-dependent variables specified in the input. Then the inlet gas conditions

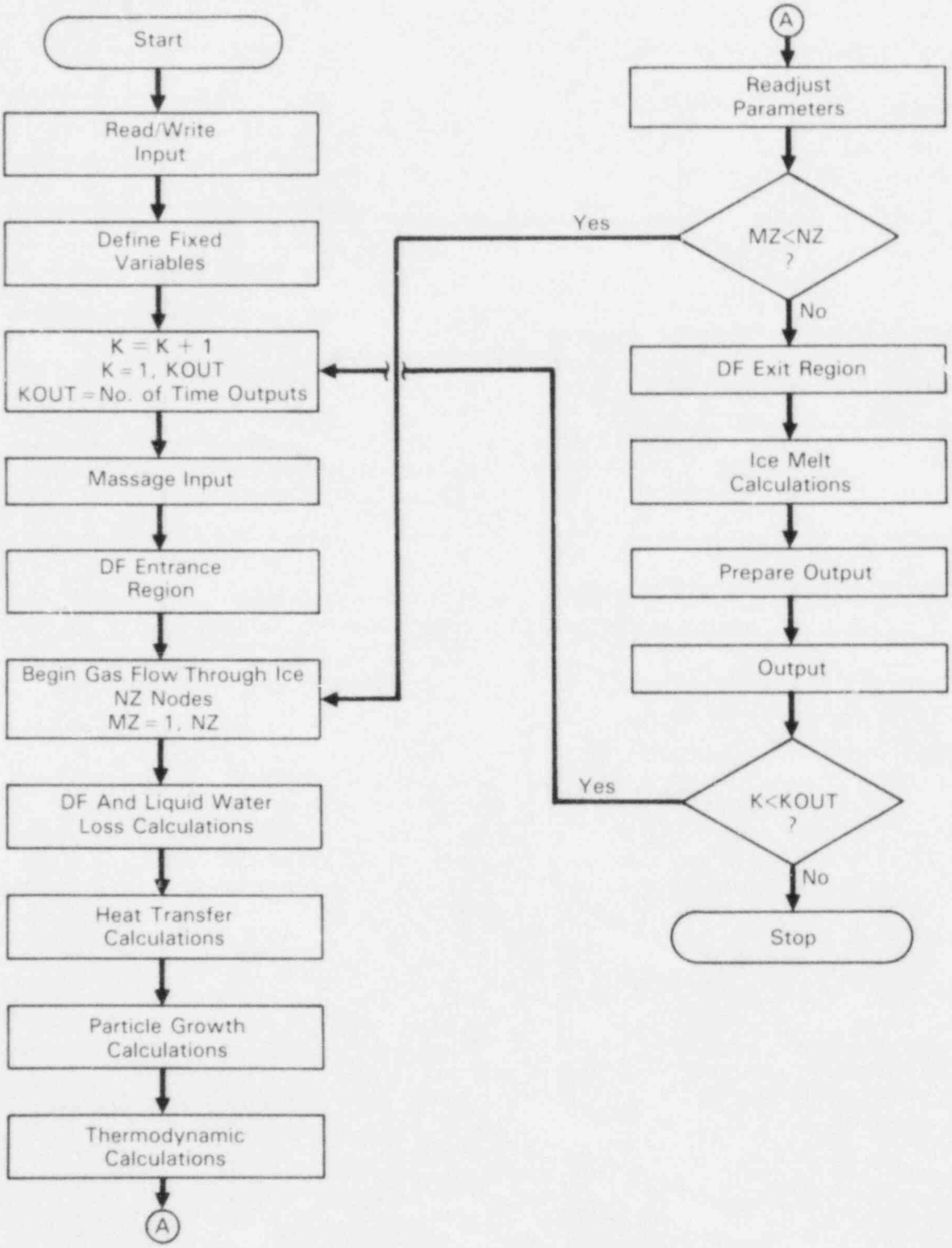

FIGURE 1. Flow Chart of the ICEDF Code

are appropriately defined for determining particle-removal rate constants for DF calculations; particle growth on soluble particles is then computed.

3.1.5 DF Entrance Region

The compartment below the ice baskets can deplete particles from the entering aerosol by gravity settling and Brownian diffusion. This is accomplished as a special well-mixed node using an appropriate form of Equation (2.15).

3.1.6 Ice Bed DO Loop

The ice bed calculations begin by following the flow in a series of NZ well-mixed nodes. The DO 290 MZ=1, NZ loop begins with the aerosol conditions leaving the entrance region at the entrance temperature.

3.1.7 DF and Liquid Water Loss Calculations

Particle loss is computed for each particle size by Equation (2.15). Then the water loss to the surfaces in the nodes via the droplets capture is calculated.

3.1.8 Heat Transfer Calculations

Both sensible and latent heat loss from the gas is computed [Equation (2.27)]. This precedes the mass and energy balances.

3.1.9 Particle Growth Calculations

In this code section, newly condensed water vapor from the previous node is placed on the airborne particles. The algorithms for this are discussed in Section 3.2.

3.1.10 Thermodynamic Calculations

The overall mass and energy balances [Equations (2.22) through (2.28)] are used to obtain an estimate of the MZ node outlet temperature without considering condensation on particles. This temperature is then readjusted to allow condensation to occur (cf., Section 3.2.2). Then the amount condensed is calculated and placed on particles in the next node.

3.1.11 Readjustment of Parameters

This section of the code returns variables indexed as outlet conditions from node MZ to inlet conditions for node MZ+1 [e.g., $\hat{E}_2$ (MZ) = $\hat{E}_1$ (MZ+1)]. At this point the calculations return to MZ = MZ + 1 if MZ + 1 $\leq$ NZ.

3.1.12 Ice Melt Calculations

These calculations are done according to subroutine ICEMELT. See Section 3.3.7.

3.1.13 DF Exit Region

This code section takes credit for removal processes that occur in the unoccupied space above the ice baskets in the same manner as the entrance region (Section 3.1.5).

3.1.14 Output Preparation

Output printing is scheduled for each TOUT (K = 1, ..., KOUT). The first output preparation consists of listing six variables at ice bed exit conditions as functions of the particle bin number J = 1, ..., 20: particle diameters both dry and wet, particle flow rate grams/second both dry and wet, particle numbers, and decontamination factor. Then 12 other quantities are prepared including number median particle radii (wet and dry), particle geometric standard deviation and integrated overall DF [Equation (2.17)]. See Section 4.3 for an example of output.

3.2 METHODS/ALGORITHMS OF CALCULATION

As mentioned in Chapter 2.0, the basis for computing DFs along the flow path is the nodalization of the flow channel into NZ nodes. Each of these nodes is considered to be well mixed; parameter values are 'lumped' for this well-mixed situation. No boundary layer phenomena exist, and all driving forces are based on a bulk gas/ice or basket surface difference. Most methods or algorithms of calculation are simple and straightforward. The more complicated methods or algorithms involving the growth of particles in supersaturated atmospheres are discussed below, along with a discussion of other model choices where alternative methods are available.

3.2.1 Heat Transfer Coefficients

For condensing steam/air mixtures on solid surfaces, the Uchida correlation for heat transfer coefficient is used (Uchida et al. 1964):

$$h_c = 0.04502\ (\rho_v/\rho_{nc})^{0.8}\ ,\ \frac{\text{watts}}{\text{cm}^2\,{}^0\text{K}} \tag{3.1}$$

with the limit

$h_c = 0.15889$ maximum.

Here ρ_v and ρ_{nc} are the vapor and noncondensible gas densities in the bulk gas. Note that other correlations are available [e.g., Handbook of Heat Transfer, p. 12-31 (Rohsenow and Hartnett 1973)].

For sensible heat transfer, more choices are available; however, the choice is made difficult by the low flow rates expected during fan flow in the ice bed channels. The Reynolds number can range typically from 3000 to 6000 for forced convection fan flow. These Reynolds numbers are in the transition region for heat transfer (Bird, Stewart and Lightfoot 1960) and present a problem for application of correlations that are good for $Re < 2100$ and $Re > 10^4$. Calculations have shown that the cold ice surfaces cause density instabilities and, therefore, natural convection flows. For this reason, a natural convection heat transfer correlation is used in ICEDF. This correlation is of the form

$$Nu_z = a \, (Gr_z Pr)^b \text{ (Jaluria 1980)} \qquad (3.2)$$

where

Nu_z = Nusselt number based on flow direction coordinate z ($o \leq z \leq \ell$)

Gr_z = Grashof number based on flow direction coordinate z

Pr = Prandtl number.

By analogy with Equation (2.11), Equation (3.2) become

$$h_s = 0.13 \, (GrPr)^{1/3} kg/\ell, \ \frac{\text{watts}}{cm^2 \cdot k} , \qquad (3.3a)$$

where the Pr is substituted for the Schmidt number Sc_j. Here

$$Pr = Cp_g \mu / kg , \qquad (3.3b)$$

where Cp_g is the gas thermal conductivity, watts/cm°K. Note that as in Equation (2.11), the transfer coefficient (here h_s) is independent of the characteristic dimension ℓ.

The version of ICEDF listed in Appendix B also uses a forced convection correlation for h_s. The source of the correlations is Figure B.2-1 in Bird 1960. The correlations developed from that figure do apply to transition Reynolds numbers, but probably with high uncertainty. h_s is obtained from equations for the plots of $NuRe_b^{-1}Pr_b^{-1/3}(\mu_b/\mu_o)^{0.14}$ versus Re_b where the subscript 'b' refers to bulk gas and o to the ice film. See subroutine IID for details of the equations used. The subroutine picks the larger h_s, either the free-convective h_s from Equation 3.3a or the forced-convective h_s above. This value of h_s is then corrected for high mass transfer rates in the manner of Bird 1960, pp. 661-664.

The well-mixed node assumption made for ICEDF ignores the three-dimensionality of the heat transfer coefficient. The Nusselt correlation type above recognizes the z (flow) direction dependence. However, the cross-section of the flow channel is cross shaped, which will give an additional two-dimensional dependence in heat transfer coefficient. The narrowest dimensions across the flow in the channel arms will have the slowest forced convection velocities and might also have the highest back flow tendencies. Experimental measurements are needed to determine the importance of this effect.

3.2.2 Particle Growth

The algorithms for calculating particle growth follow the sequence of events below for each node:

1. Calculate T(2), the node temperature, without allowing for condensation to occur.
2. Calculate apparent saturation, S. If $S > 1$, continue.
3. Calculate new T'(2) for $S' = 1$ that allows DXI, g moles/s to condense on particles. This is the thermodynamic maximum growth rate. This computation is done by intersecting two lines obtained from DXI = DXI $[\rho_v, T'(2)]$ and DXI = DXI $[\dot{E}, T'(2)]$, and solving for DXI and T'(2).
4. Use Mason's equation (2.21) with above S and the Kelvin restriction to calculate the maximum growth rate, DXS, for all particles in the node.
5. If DXS > DXI, then the thermodynamic growth rate limit applies. If DXS < DXI, then the particle growth rate equation applies; go to 7.
6. For DXS > DXI, the particles are allowed to share DXI in the following way: An equation for approximating small mass increases in a droplet can be obtained from Mason's equation (2.20):

$$\Delta M_j = 2\pi dp_j (S - S')\rho_L \ \Delta t/(a+b) \ , \qquad (3.4)$$

where

ΔM_j = mass of particle size j increase, g

dp_j = original diameter, cm

Δt = time of growth, s.

If $\dot{n}_j$ = mass flow rate of particle size j out the node, then the total growth rate for all particles is

$$18DXI = \sum_{j=j'}^{20} \dot{n}_j \Delta m_j = \left[2\pi \, (S-S')\rho_L \; \Delta t/(a+b)\right] \sum_{j=j'}^{20} \dot{n}_j \, dp_j \quad (3.5)$$

where j' = smallest j where particles are allowed to grow (Kelvin restriction)

or

$$18 \, DXI = A \sum_{j=j'}^{20} \dot{n}_j \, dp_j \; . \quad (3.6)$$

Since the true value of S is not known when growth is limited by thermodynamic principles, the value of A is found by Equation (3.6); then each particle grows by $\Delta M_j = Adp_j$ in the node.

7. For DXS < DXI, the particle growth per particle is obtained by Equation (2.21). This situation only occurs when few particles remain in the gas phase. The expressions for the constants a and b in Equation (2.21) are estimated by curves in Byers 1965. These curves can be expressed approximately as

$$a = \exp\left[1.35008 - 1.11063E\text{-}02 \; (T - 273.2)\right] \quad (3.7)$$

$$b = \exp\left[13.7102E\text{-}06 - 6.45E\text{-}02 \; (T - 273.2)\right] \quad (3.8)$$

where T = actual temperature, °K.

3.3 SUBROUTINES

The following seven subroutines support the main program.

3.3.1 Subroutine KELVIN

This subroutine determines if particles can grow under the restrictions of the Kelvin equation (see footnote, p. 10). If the vapor pressure of a curved droplet exceeds that of the surrounding vapor, growth is not permitted. For the smaller droplets, which have a curvature that permits growth, curvature still hinders growth.

3.3.2 Subroutine DIFFU

This subroutine computes the Brownian diffusion coefficient, D_j, in cm^2/s as a function of particle size, j, the mean free path of gas molecules, λ, in cm, and the Cunningham slip factor, Cn_j. Here

$$D_j = 1.38E\text{-}16\ T\ Cn_j/(3\pi\mu d_p),\ \text{cm}^2/\text{s} \tag{3.9}$$

$$Cn_j = 1 + 2.492 \frac{\lambda}{dp_j} + 0.84 \frac{\lambda}{dp_j} \exp\left(-0.435 \frac{dp_j}{\lambda}\right),\ \text{dimensionless} \tag{3.10}$$

$$\lambda = 1.245E\text{-}02\ (T/Mw)^{0.5}\ \mu/P\ , \tag{3.11}$$

where

P = absolute gas pressure, atm.

3.3.3 Subroutine VISC

This subroutine computes the viscosity of the gas mixture in poises and thermal conductivity of the gas mixture in watts/cm°K. Individual gas viscosities are calculated from Bird, Stewart and Lightfoot (1960):

$$\mu_i = 2.6693E\text{-}5\ \sqrt{Mw_i\ T}/\sigma_i^2\ \Omega_i,\ \text{poise} \tag{3.12}$$

where

σ_i = collision diameter of molecules

$\Omega_i = \Omega_i\ (kT/\varepsilon_i)$

ε_i = Lennard-Jones 'well' energy.

and viscosity of the mixture is also from Bird, Stewart and Lightfoot (1960):

$$\mu_{mix} = \sum_{i=1}^{n} \frac{X_i \mu_i}{\sum_{j=1}^{n} X_i\ \Phi_{ij}} \tag{3.13}$$

$$\Phi_{ij} = \frac{1}{\sqrt{8}}\left(1 + \frac{Mw_i}{Mw_j}\right)^{-1/2}\left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2}\left(\frac{Mw_j}{Mw_i}\right)^{1/4}\right]^2 \qquad (3.14)$$

The thermal conductivity is calculated using similar equations.

3.3.4 Subroutine VSET

This subroutine computes the terminal settling velocity of a particle in a gas phase. The method uses the Stokes settling equation:

$$V_j = \rho G C n_j dp_j^2 \;/\; 18\mu \qquad (3.15)$$

for $f_{Re} < 9.6$ where

$$f_{Re} = \frac{4}{3}\rho\rho_j G dp_j^3/\mu^3 \;. \qquad (3.16)$$

For larger f_{Re}, empirical expressions are used in ICEDF for $Re_j = Re_j\ (f_{Re})$ where Re_j = Reynolds number $\rho dp_j V_j/\mu$ (Knudsen 1970).

3.3.5 Subroutine IID

This subroutine calculates the Brownian diffusion coefficient of Equation (2.11), the impaction/interception efficiency ε_I of Equation (2.7), the Brownian diffusion efficiency ε_{BD_j} of Equation (2.9), and the convective heat transfer coefficient, h_s [see 3.2.1].

3.3.6 Subroutine SOLGRO

This subroutine computes the diameter multiplier, $RDPART_j$, the growth factor for soluble particles using a simplified form of Equation (2.29), assuming that the soluble fraction of the dry particle is C_sOH. In the main code

$$dp_j = RDPART_j \times DPART_j,\ \text{cm}\ , \qquad (3.17)$$

where $DPART_j$ = original dry particle diameter as a sphere.

3.3.7 Subroutine ICEMELT

This subroutine calculates the amount of ice remaining in the ice bed as a function of time. Enthalpy and mass balances are solved about the total ice bed using the exit gas temperature and composition calculated in the manner found in Section 2.2.1. The water leaving the bottom of the bed is assumed to be at the entering gas temperature and the ice shape is assumed to be cylindrical, diminishing in diameter as the ice melts. ICEMELT also estimates water film thickness and temperature on the ice for heat transfer calculations. An improved version of ICEMELT is expected to be developed, which will use actual ice geometry and water film thicknesses based on local heat transfer.

4.0 CODE OPERATION AND PARAMETER SELECTION

Code ICEDF has been written in FORTRAN-IV with some use of FORTRAN 77. The input file uses the free format of FORTRAN 77. This chapter details the necessary input requirements of the code and gives output description along with examples of both input and output. Parameter guidance is given in Section 4.1.1 and 4.1.2.

4.1 INPUT REQUIREMENTS

The input file of ICEDF requires three types of information: 1) ice bed physical parameters, 2) inlet aerosol parameters, and 3) calculational and output specifications.

4.1.1 Ice Bed Physical Parameters

For a detailed description of typical PWR ice bed parameters, see Winegardner et al. (1983). The necessary ICEDF parameters are also discussed. The code has a number of fixed ice bed parameters: AX, NUNIT, PERIM, and DZL. Examples of each follow:

AX = cross-sectional area, cm^2, of the single flow channel between ice basket columns (e.g., 565.4)

NUNIT = number of flow channels per reactor (e.g., 1944)

PERIM = 'wetted' perimeter of a single flow cross section, cm (e.g., 95.8)

DZL = length of a flow channel, cm (e.g., 1460).

These can be changed at the user's preference, but require recompilation.

Ice bed physical parameters that must be specified in each run are

NDATA = number of data entry points per run where input parameters are specified

TI(J) = time values (minutes) of each data entry point, J=1, NDATA

EF = factor used in the definition of ice surface area, based on the fraction of basket volume filled with solid ice and the fraction of the initial surface area exposed to gas

AS1 = basket sedimentation area, cm^2

AS2 = ice sedimentation area, cm^2

AS3 = floor sedimentation area, cm^2

AS4 = upper compartment sedimentation area, cm^2

AI1 = basket impaction area, cm^2

AI2 = ice impaction area, cm^2

AD1 = basket diffusion area, cm^2

AD2 = ice diffusion area, cm^2

AD3 = floor diffusion area, cm^2

AD4 = upper compartment diffusion area, cm^2.

Typical values of the above that can be used are

NDATA = 2 (minimum) to 50 (dimension limit)

TI(J), J=1, NDATA = 0.,......

EF = 0. →0.3

AS1 = 2.2E+07 cm^2

AS2 = 1.25E+10 cm^2

AS3 = 4.E+06 cm^2

AS4 = 4.E+06 cm^2

AI1 = 1.24E+07 cm^2

AI2 = 0.

AD1 = 3.43E+07 cm^2

AD2 = 2.5E+10 cm^2

AD3 = 3.1E+08 cm^2

AD4 = 1.6E+08 cm^2.

Assuming ice is in the form of flakes and considering removal by sedimentation, Winegardner et al. (1983) give reasons for selecting 0.3 as a possible upper bound for the parameter EF. Since the ice can fuse (glaciate) prior to any accident and can melt during an accident, this value probably is too high. A more realistic value for a column of new ice flakes that allows gas penetration to ~1 cm gives EF ~0.05, which might be a good starting point. Experimental measurements and/or observations at existing reactors are needed to provide a better definition of EF.

4.1.2 Inlet Aerosol Parameters

Definition of particle as well as bulk gas characteristics is needed to develop values for inlet aerosol parameters. Since inlet particle size is probably the most important parameter in the ICEDF code, considerable effort should be made to specify the size distribution throughout the accident sequence. There are 20 particle sizes specified in a DATA DPART/..../ statement. These 20 sizes can be a discrete representation of a particle-size distribution, as is shown in the listing example (Appendix B, line 0050). The example represents a lognormal distribution around a mass median diameter (MMD) of 1.0E-04 cm (1 μm). That DATA DPART statement combined with the following input vector for PARCON (J,I)

PARCON (1,I) = 8.00E-10
PARCON (2,I) = 2.95E-09
PARCON (3,I) = 9.75E-09
PARCON (4,I) = 2.65E-08
PARCON (5,I) = 7.50E-08
PARCON (6,I) = 1.65E-07
PARCON (7,I) = 2.95E-07
PARCON (8,I) = 4.75E-07
PARCON (9,I) = 7.00E-07
PARCON (10,I) = 7.50E-07
PARCON (11,I) = 7.50E-07
PARCON (12,I) = 7.00E-07
PARCON (13,I) = 4.75E-07
PARCON (14,I) = 2.95E-07
PARCON (15,I) = 1.65E-07
PARCON (16,I) = 7.50E-08
PARCON (17,I) = 2.65E-08
PARCON (18,I) = 9.75E-09
PARCON (19,I) = 2.95E-09
PARCON (20,I) = 8.00E-10

complete an inlet particle-size distribution at time TI(I) with a geometric standard deviation $\sigma_g = 2$ and a total inlet particle concentration of 5E-06 g/cm^3 at the inlet gas conditions. To change the MMD by a certain factor at input time TI(I), specify the factor by DMULT(I). To change the particle concentrations by a single factor, specify the factor by PMULT(I). If the user desires to change σ_g, each PARCON (J,I) must be changed. It is easy to set σ_g to $\sigma_g = \infty$ where each PARCON (J-1,I) = PARCON (J,I) = PARCON (J+1,I) and to $\sigma_g = 1$ where only one PARCON (J,I) $\neq$ 0. To adjust the PARCON vector to accommodate other σ_g values, a set of computations are necessary that are too extensive to be explained here. (Refer to any fundamental treatise on aerosols.)

Other properties of the aerosol particle required as input are

RHO(I) = particle density, g/cm^3, I=1, NDATA

SOLF(I) = weight fraction of dry mass that is water soluble, I=1, NDATA.

Values of RHO(I) are typically 1.0 g/cm^3 for dilute aqueous droplets to as high as 11.0 g/cm^2 for fuel particles as UO_2. Values for SOLF(I) range from zero for insoluble masses to 1.0 for dry masses consisting entirely of soluble compounds such as CsI or CsOH.

The final requirements for aerosol specifications involve the carrier gas description. These are

TGASIN(I) = inlet gas temperature, °C, I=1, NDATA

PGASIN(I) = absolute pressure of inlet gas, atm, I=1, NDATA

XH2I(I) = hydrogen mole fraction of inlet gas, I=1, NDATA

XH2OI(I) = water vapor mole fraction of inlet gas, I=1, NDATA

QUALI(I) = quality of inlet water, %, I=1, NDATA

XOH2OI(I) = water vapor mole fraction of exiting gas, I=1, NDATA

XCOI(I) = carbon monoxide mole fraction of inlet gas, I=1, NDATA

XCO2I(I) = carbon dioxide mole fraction of inlet gas, I=1, NDATA

XAIRI(I) = air mole fraction of inlet gas, I=1, NDATA

TGSOUT(I) = temperature of exit gas, °C, I=1, NDATA

GASINI(I) = gas inlet rate, m^3/s, I=1, NDATA.

Normally QUALI(I) = 100. Rarely will sufficient liquid water be entrained in the inlet gas for this parameter to be another value; e.g., a cold fog might qualify as a possible situation for QUALI(I) < 100.

Values for XOH2OI(I) and TGSOUT(I) are calculated by the code as the gas flows toward the exit. However, rough estimates are needed initially. For a full ice bed, XOH2OI(I) = 0.006 and TGSOUT(I) = 0. For an empty ice bed, XOH2OI(I) = XH2OI(I), and TGSOUT(I) = TGASIN(I).

4.1.3 Calculational and Output Specifications

Only four input numbers are required in this category: 1) NZ, the number of calculational nodes (see Section 2.1); 2) MICE, the ice melt switch; 3) KOUT, the desired number of times of output at 4) TOUT (K, K=1, KOUT) minutes (see Section 3.1.3.).

NZ controls the accuracy of calculations and represents the degree of backmixing. NZ > 200 seems to give sufficient resolution of the gas temperature profile. However, if no ice is present, a lower NZ should give adequate

DF resolution. For extremely slow flow rates, an even larger NZ might be necessary. No default limits on NZ as a function of GASIN have been determined. Future experiments might provide better guidelines for NZ.

MICE is a switch to allow the ice to melt. If MICE = 0, no melting is allowed. This is useful for parametric studies where the quantity of ice is to be fixed. If MICE $\neq$ 0, then ice is allowed to melt according to the ICEMELT subroutine. XMICE is the fraction of unmelted ice at TI(1) = 0.

KOUT and TOUT (K, K = 1, KOUT) are the output controls. KOUT must be >1 and TOUT (1) = 0. When ice is melting, it might be desirable to set KOUT > 10 and pick the TOUT(K)s to correspond to the TI(J)s as well as to fill in any time regions of rapidly changing conditions. Also TOUT(2) $\leq$1 min will allow the ice bed to respond to the early presence of melt water.

4.2 OUTPUT DESCRIPTION

The currently programmed output consists of two parts: the 'echo' of the input file and the output calculated for each time step TOUT(K). The calculated output also consists of two parts: the essential particle-size distribution information at the ice bed outlet, and other information on the overall particle distribution and gas conditions at the outlet. These are described in Sections 4.2.1 and 4.2.2 and exhibited in Section 4.3.

4.2.1 Output Description by Particle Size

The output file per time step is headed by a TOUT(K) print and 'Materials Leaving Ice Bed.' Below this is a matrix of eight vertical 20-component vectors of these material for each particle size:

1. Particle bin number
2. Particle dry diameter (cm)
3. Wet particle diameter (cm)
4. Particle flow rate, dry (g/s)
5. Particle mass flow rate, wet (g/s)
6. Particle number flow rate, particles/s
7. Particle decontamination factor
8. Containment particle removal rate constant, 1/s.

4.2.2 Additional Output

For the same TOUT(K), 16 other outlet (unless otherwise noted) variables are printed:

1. Individual particle density, dry (g/cm^3)
2. Individual particle density, wet (g/cm^3)
3. Weight fraction of water in particles
4. Number median dry particle radius, cm
5. Number median wet particle radius, cm
6. σ_g for dry particles
7. σ_g for wet particles
8. Mass flow rate of dry particles into the ice bed (g/s)
9. Mass flow rate of dry particles leaving the ice bed (g/s)
10. Mass flow rate of wet particles leaving the ice bed (g/s)
11. Integrated decontamination factor (No. 8/No. 9)
12. Total particle flow rate leaving the bed, including condensed water, g/s
13. Gas outlet relative humidity, percent
14. Gas outlet temperature, °C
15. Removal rate constant for all particles based on containment volume, 1/s
16. Fraction of initial ice remaining.

4.3 INPUT/OUTPUT EXAMPLES

Figures 2 and 3 are examples of an input file and the output echo of that input file, respectively. The unique feature of this input file is that it demonstrates the ICEMELT subroutine through the almost complete melting of the full charge of ice. The ice was nearly melted by 18.3 h of constant 100°C air/steam flow. DFjs for the larger particles are attenuated several orders of magnitude from the initial values with a full charge of ice to those at 18.3 h.

Figures 4 and 5 are examples of the output described on Sections 4.2.1 and 4.2.2. previously. These examples are the 18.3-h output by particle size and the overall properties of the aerosol at 18.3 h for Figure 2 input file. For brevity, no comparisons with output values at earlier times are given.

```
4
0.,275.,550.,1100.
1.,1.,1.,1.
0.0,0.0,0.0,0.0
8.E-10,8.E-10,8.E-10,8.E-10
2.95E-9,2.95E-9,2.95E-9,2.95E-9
9.75E-9,9.75E-9,9.75E-9,9.75E-9
2.65E-8,2.65E-8,2.65E-8,2.65E-8
7.5E-8,7.5E-8,7.5E-8,7.5E-8
1.65E-7,1.65E-7,1.65E-7,1.65E-7
2.95E-7,2.95E-7,2.95E-7,2.95E-7
4.75E-7,4.75E-7,4.75E-7,4.75E-7
7.E-7,7.E-7,7.E-7,7.E-7
7.5E-7,7.5E-7,7.5E-7,7.5E-7
7.5E-7,7.5E-7,7.5E-7,7.5E-7
7.E-7,7.E-7,7.E-7,7.E-7
4.75E-7,4.75E-7,4.75E-7,4.75E-7
2.95E-7,2.95E-7,2.95E-7,2.95E-7
1.65E-7,1.65E-7,1.65E-7,1.65E-7
7.5E-8,7.5E-8,7.5E-8,7.5E-8
2.65E-8,2.65E-8,2.65E-8,2.65E-8
9.75E-9,9.75E-9,9.75E-9,9.75E-9
2.95E-9,2.95E-9,2.95E-9,2.95E-9
8.E-10,8.E-10,8.E-10,8.E-10
100.,100.,100.,100.
1.,1.,1.,1.
0.,0.,0.,0.
100.,100.,100.,100.
.2,.2,.2,.2
.006,.006,.006,.006
0.,0.,0.,0.
0.,0.,0.,0.
.8,.8,.8,.8
0.,0.,0.,0.
32.25,32.25,32.25,32.25
1.,1.,1.,1.
1.,1.,1.,1.
1.,1.,1.,1.
2.2E+7,1.25E+10,4.E+6,4.E+6,1.24E+7,0.,3.43E+7,2.5E+10,3.1E+8,1.6E+8
200,2.16,1.,4,1.E+11,1,1.,.05
0.,275.,550.,1100.
```

FIGURE 2. Example of an Input File

```
NDATA=           4
TI(I)=  0.0000000E+00   275.0000        550.0000        1100.000
RHO(I)=   1.000000        1.000000        1.000000        1.000000
SOLF(I)=  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
PARCON(J,I)=  8.0000001E-10  8.0000001E-10  8.0000001E-10  8.0000001E-10
PARCON(J,I)=  2.9500000E-09  2.9500000E-09  2.9500000E-09  2.9500000E-09
PARCON(J,I)=  9.7499999E-09  9.7499999E-09  9.7499999E-09  9.7499999E-09
PARCON(J,I)=  2.6500000E-08  2.6500000E-08  2.6500000E-08  2.6500000E-08
PARCON(J,I)=  7.5000003E-08  7.5000003E-08  7.5000003E-08  7.5000003E-08
PARCON(J,I)=  1.6500000E-07  1.6500000E-07  1.6500000E-07  1.6500000E-07
PARCON(J,I)=  2.9500001E-07  2.9500001E-07  2.9500001E-07  2.9500001E-07
PARCON(J,I)=  4.7500001E-07  4.7500001E-07  4.7500001E-07  4.7500001E-07
PARCON(J,I)=  6.9999999E-07  6.9999999E-07  6.9999999E-07  6.9999999E-07
PARCON(J,I)=  7.5000003E-07  7.5000003E-07  7.5000003E-07  7.5000003E-07
PARCON(J,I)=  7.5000003E-07  7.5000003E-07  7.5000003E-07  7.5000003E-07
PARCON(J,I)=  6.9999999E-07  6.9999999E-07  6.9999999E-07  6.9999999E-07
PARCON(J,I)=  4.7500001E-07  4.7500001E-07  4.7500001E-07  4.7500001E-07
PARCON(J,I)=  2.9500001E-07  2.9500001E-07  2.9500001E-07  2.9500001E-07
PARCON(J,I)=  1.6500000E-07  1.6500000E-07  1.6500000E-07  1.6500000E-07
PARCON(J,I)=  7.5000003E-08  7.5000003E-08  7.5000003E-08  7.5000003E-08
PARCON(J,I)=  2.6500000E-08  2.6500000E-08  2.6500000E-08  2.6500000E-08
PARCON(J,I)=  9.7499999E-09  9.7499999E-09  9.7499999E-09  9.7499999E-09
PARCON(J,I)=  2.9500000E-09  2.9500000E-09  2.9500000E-09  2.9500000E-09
PARCON(J,I)=  8.0000001E-10  8.0000001E-10  8.0000001E-10  8.0000001E-10
TGASIN(I)=   100.0000        100.0000        100.0000        100.0000
PGASIN(I)=   1.000000        1.000000        1.000000        1.000000
XH2I(I)=  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
QUALI(I)=  100.0000        100.0000        100.0000        100.0000
XH2OI(I)=  0.2000000       0.2000000       0.2000000       0.2000000
XOH2OI(I)=  6.0000001E-03  6.0000001E-03  6.0000001E-03  6.0000001E-03
XCOI(I)=  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
XCO2I(I)=  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
XAIRI(I)=  0.8000000       0.8000000       0.8000000       0.8000000
TGSOUT(I)=  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00
GASINI(I)=   32.25000        32.25000        32.25000        32.25000
CHII(I)=  1.000000        1.000000        1.000000        1.000000
 PMULT(I)=   1.000000        1.000000        1.000000        1.000000
 DMULT(I)=   1.000000        1.000000        1.000000        1.000000
 AS1=  2.2000000E+07 AS2=  1.2500000E+10 AS3=   4000000.     AS4=   4000000.
 AI1=  1.2400000E+07 AI2=  0.0000000E+00 AD1=  3.4300000E+07 AD2=  2.4999999E+10
 AD3=  3.1000000E+08 AD4=  1.6000000E+08
 NZ=          200 CT=   2.160000     CMOM=   1.000000     KOUT=           4
 VOLCON=  9.9999998E+10 MICE=            1 XICE=   1.000000     EF= 5.0000001E-02
TOUT(K)=  0.0000000E+00   275.0000        550.0000        1100.000
```

FIGURE 3. ICEDF Printout of Figure 2 Input File

```
TOUT(004)=1100.00 MINUTES. MATERIALS LEAVING ICEBED


PARTICLE  PARTICLE     PARTICLE      GRAMS        GRAMS       NUMBER       DECON.       LAMBDA
  BIN       DIAM         DIAM       PER SEC      PER SEC      PER SEC      FACTOR       1/SEC
NUMBER    DRY (CM)     WET (CM)       DRY          WET                       DF

   1      0.7600E-05  0.7600E-05  0.2062E-01  0.2062E-01  0.8971E+14  0.1251E+01  0.6474E-04
   2      0.1000E-04  0.1000E-04  0.7592E-01  0.7592E-01  0.1450E+15  0.1253E+01  0.6515E-04
   3      0.1300E-04  0.1300E-04  0.2505E+00  0.2505E+00  0.2177E+15  0.1255E+01  0.6562E-04
   4      0.1700E-04  0.1700E-04  0.6792E+00  0.6792E+00  0.2640E+15  0.1258E+01  0.6620E-04
   5      0.2200E-04  0.2200E-04  0.1917E+01  0.1917E+01  0.3439E+15  0.1261E+01  0.6685E-04
   6      0.3000E-04  0.3000E-04  0.4203E+01  0.4203E+01  0.2973E+15  0.1266E+01  0.6775E-04
   7      0.3900E-04  0.3900E-04  0.7489E+01  0.7489E+01  0.2411E+15  0.1270E+01  0.6863E-04
   8      0.5200E-04  0.5200E-04  0.1201E+02  0.1201E+02  0.1631E+15  0.1276E+01  0.6973E-04
   9      0.6800E-04  0.6800E-04  0.1761E+02  0.1761E+02  0.1070E+15  0.1282E+01  0.7093E-04
  10      0.8400E-04  0.8400E-04  0.1878E+02  0.1878E+02  0.6053E+14  0.1288E+01  0.7204E-04
  11      0.1100E-03  0.1100E-03  0.1865E+02  0.1865E+02  0.2677E+14  0.1297E+01  0.7378E-04
  12      0.1500E-03  0.1500E-03  0.1722E+02  0.1722E+02  0.9743E+13  0.1311E+01  0.7654E-04
  13      0.2000E-03  0.2000E-03  0.1150E+02  0.1150E+02  0.2746E+13  0.1332E+01  0.8037E-04
  14      0.2600E-03  0.2600E-03  0.6987E+01  0.6987E+01  0.7592E+12  0.1362E+01  0.8566E-04
  15      0.3500E-03  0.3500E-03  0.3752E+01  0.3752E+01  0.1671E+12  0.1418E+01  0.9513E-04
  16      0.4500E-03  0.4500E-03  0.1611E+01  0.1611E+01  0.3377E+11  0.1501E+01  0.1077E-03
  17      0.5900E-03  0.5900E-03  0.5128E+00  0.5128E+00  0.4769E+10  0.1666E+01  0.1290E-03
  18      0.7800E-03  0.7800E-03  0.1401E+00  0.1401E+00  0.5639E+09  0.2244E+01  0.1788E-03
  19      0.9500E-03  0.9500E-03  0.3001E-01  0.3001E-01  0.6685E+08  0.3170E+01  0.2208E-03
  20      0.1030E-02  0.1030E-02  0.6777E-02  0.6777E-02  0.1185E+08  0.3807E+01  0.2378E-03
```

FIGURE 4. Particle-Size of Output for Figure 2 Input File at 18.3 h

```
0.1000E+01  DRY PARTICLE DENSITY (GM/CM**3)
0.1000E+01  WET PARTICLE DENSITY (GM/CM**3)
0.0000E+00  WEIGHT FRACTION WATER IN PARTICLES
0.1249E-04  NUMBER MEDIAN PARTICLE RADIUS OF DRY PARTICLES (CM)
0.1249E-04  NUMBER MEDIAN PARTICLE RADIUS OF WET PARTICLES(CM)
0.1990E+01  GEOMETRIC STANDARD DEVIATION OF DRY PARTICLES
0.1990E+01  GEOMETRIC STANDARD DEVIATION OF WET PARTICLES
0.1613E+03  TOTAL GRAMS/SEC DRY PARTICLES INTO ICEBED
0.1234E+03  TOTAL GRAMS/SEC DRY PARTICLES LEAVING ICEBED
0.1306E+01  INTEGRATED DECONTAMINATION FACTOR
0.1234E+03  TOTAL GRAMS/SEC WET PARTICLES LEAVING ICEBED
0.1000E+03  RELATIVE HUMIDITY OF GAS LEAVING ICEBED (PERCENT)
0.1495E-02  OUTLET GAS TEMPERATURE (DEG C)
0.7560E-04  REMOVAL LAMBDA FOR ALL PARTICLES (1/SEC)
0.5219E-01  FRACTION OF INITIAL ICE REMAINING
```

FIGURE 5. Overall Aerosol Properties Part of the Output File for Figure 2 Input File at 18.3 h

5.0 CODE VALIDATION STATUS

The ICEDF code was independently reviewed and documented in February 1984 (Kress 1984). This chapter summarizes that review and briefly describes validation experiments that are being planned.

5.1 ICEDF VALIDATION STATUS REVIEW

The above-mentioned code review used NUREG/CR-3248 (see Section 2.1) as the source of information on the technical bases for the ICEDF code. The most significant comments from this review are as follows: 1) Equation (2.15) would underpredict overall particle DFs for unidirectional flow. The problem remains that the degree of backmixing on the ice bed flow is not known. A three-dimensional flow analysis is needed to determine if the assumed series of well-mixed nodes used in deriving Equation (2.15) is more sound than a unidirectional flow model (not used in ICEDF). 2) The nearly total absence of supporting data makes systematic validation currently impossible. There are data, however, on each individual removal mechanism used in ICEDF. These data give support to their use in ICEDF; however, no data exist that include all the mechanisms together that were obtained with ice of proper dimensions and with expected flow conditions of an accident. Some of these data will be obtained in the planned tests described in Section 5.2.

5.2 VALIDATION EXPERIMENTAL PLANS

Work has already begun on the first of a progressive series of tests to develop validation data for the ICEDF computer code. Because of the numerous variables involved, the experimental plan has been initiated with small-scale, lower-cost laboratory studies. Initial results, along with additional calculations and experimental design, will then be used in the development of larger-scale prototype test facilities.

As suggested above, the major purposes of the laboratory studies are to refine experimental techniques and ensure that focus is on key parameters prior to developing larger-scale experiments. The laboratory test apparatus is shown schematically in Figure 6. Solid particles are generated by nebulizing and drying solutions of water-soluble materials or liquid suspensions of monodisperse polystyrene latex spheres. Polydisperse aerosols can be further classified and sorted into essentially monodisperse distributions by techniques based on electrical mobility. Aerosols of the desired properties are then directed past a cylindrical deposition target. Particle-capture mechanisms will be isolated and quantitatively evaluated by first operating with a dummy target to establish the extent of background retention by direct capture mechanisms (e.g., interception, impaction, and/or Brownian diffusion). The dummy target will then be replaced by a cold finger or ice target to supplement collection by thermophoresis. Finally, steam will be introduced to add retention by diffusiophoresis and to investigate condensational particle growth. Optical light-scattering techniques are used for measurements of the concentration and particle size of effluent aerosols.

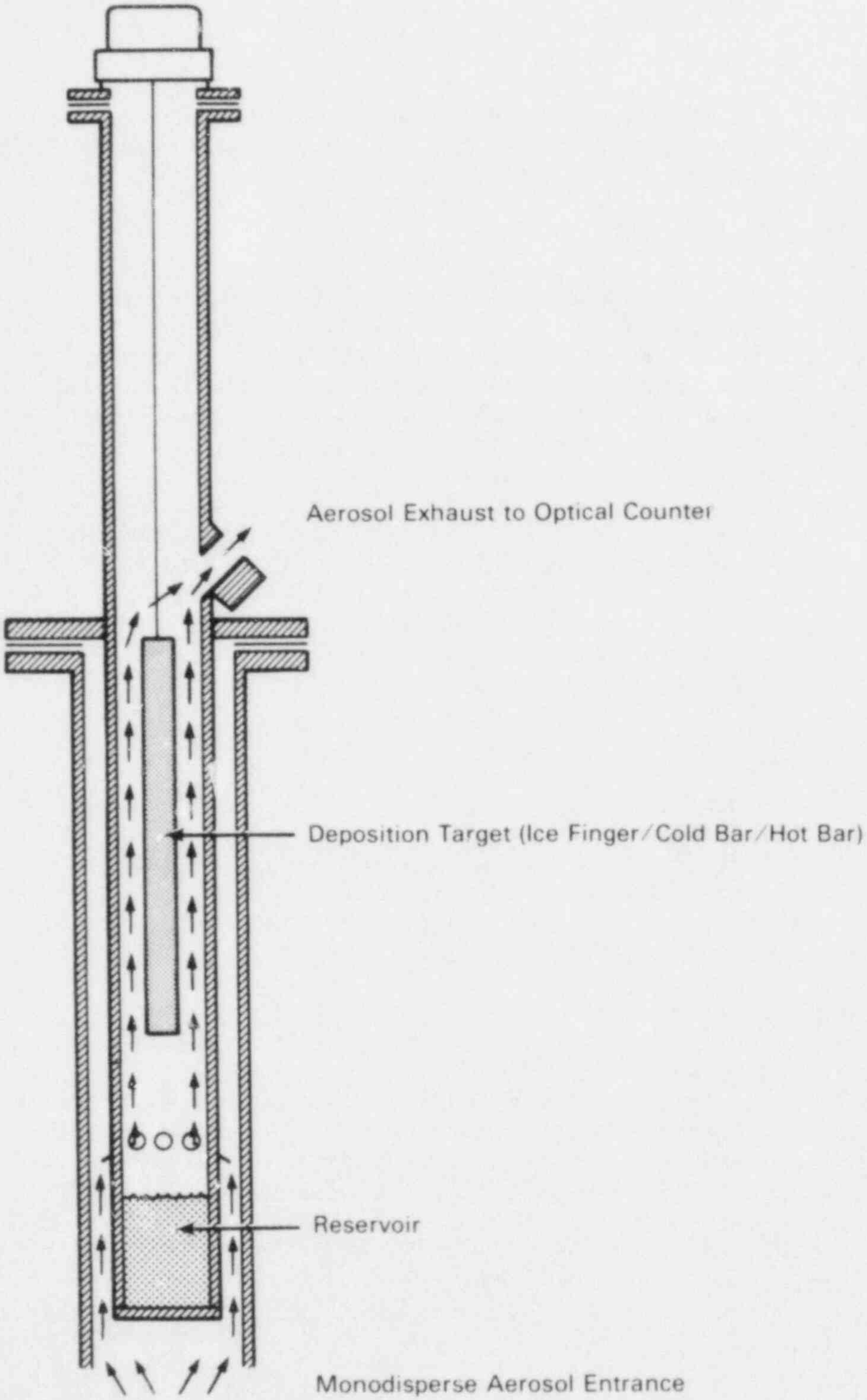

FIGURE 6. Ice Condenser Validation Tests, Phase I Laboratory Apparatus

Current plans are to follow the first-phase laboratory investigations with tests using a more prototypic vertical wind tunnel. The purpose of these tests will be to better define boundary geometries (e.g., flow around ice baskets, geometries available for deposition) for the phenomenological models that have been developed. Investigation of particle behavior would include the verification of predictions based on combined growth and retention phenomena as well as the characterization of individual mechanisms. A possible test section geometry, based on a single ice basket and sections of ice baskets, is shown in Figure 7. The basket would be placed in a housing to simulate the gas space associated with the test ice basket out to the surfaces of the adjacent baskets. Exterior surfaces of the housing would be insulated. Air as well as air-steam mixtures would be used. Ice would be loaded manually prior to each test. Length of the test section expected to be about 25 ft ultimately will be dictated by additional calculations concerning expected flow patterns and condensation rates.

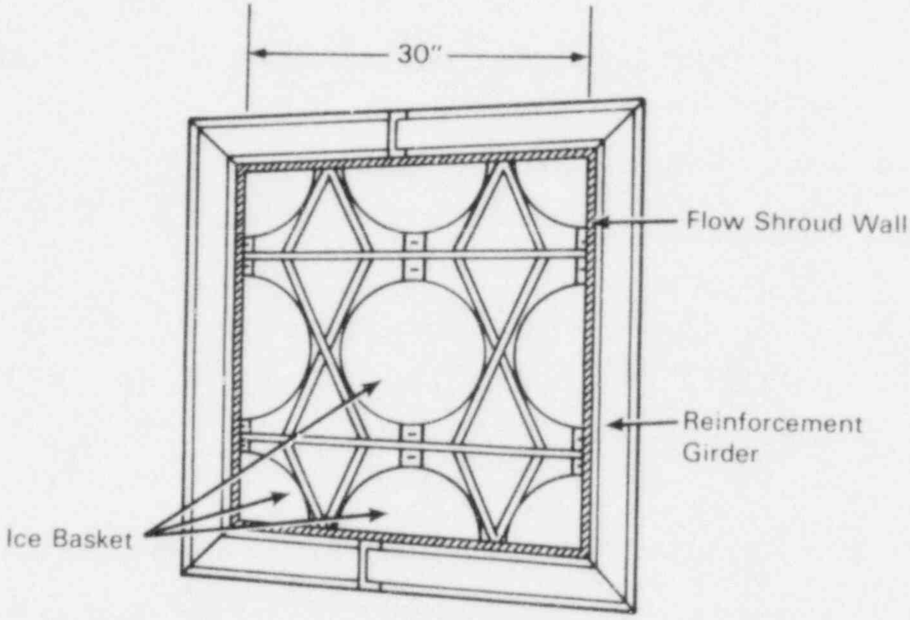

FIGURE 7. Ice Condenser Validation Tests, Cross Section of Single Basket Test Apparatus

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APPENDIX A

PARAMETER AND MECHANISM SENSITIVITY

APPENDIX A

PARAMETER AND MECHANISM SENSITIVITY

This appendix summarizes parameter and mechanism sensitivities in the ICEDF code. With this summary, the user can concentrate on the most important controlling parameters in specifying code input and can better understand the calculated DFs in terms of mechanisms modeled in the code.

In Owczarski (1984a) a sensitivity study ranked the parameters without condensation occurring on particles. A later paper (Owczarski 1984b) included the effects of condensation. Table A.1 was constructed from the two papers for the ranking of the controlling parameters:

TABLE A.1. Parameter Sensitivity Summary

Most Important
- Particle-size distribution

Very Important
- Particle-inlet concentration
- Ice availability
- Inlet steam mole fraction
- Particle density

Moderately Important
- Inlet gas flow rate
- Particle solubility
- Noncondensible gas species
- Inlet gas temperature

Least Important
- Inlet gas pressure

These parameters are not independent. Particle-inlet concentration is only important if the inlet steam mole fraction is high, which requires a fairly high inlet gas temperature. If sufficient ice is present, then condensation can occur, usually resulting in enhanced DFs.

Owczarski (1984a) ranks the importance of the removal mechanisms for a given base case. If the ice compartment is fully charged, diffusiophoresis and particle settling are the most important mechanisms. Impaction/interception are only important at very high flow rates and for large particles; thermophoresis is important only at high inlet gas temperatures. Brownian diffusion becomes important only for particles <0.1 μm diameter.

REFERENCES

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APPENDIX B

ICEDF LISTINGS

APPENDIX B

ICEDF LISTINGS

```
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C       DRAFT VERSION OF CODE ICEDF IN DEVELOPMENT
C       TO MODEL ICE CONDENSER AEROSOL REMOVAL.
C
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
c       This code has been prepared in contemplation of Commission action.
c       It may not have received patent review and may contain information
c       received in confidence.  Therefore, the contents of this code
c       should neither be disclosed to others nor reproduced wholly or
c       partially, unless written permission to do so has been obtained
c       from the appropriate U.S. NRC office.  The recipient is requested
c       to take the necessary action to ensure the protection of this code.
c       The distribution of the computer code is governed by the 'industrial
c       property of a proprietary nature' clause of the Article on 'Use of
c       Information' of the Agreement on Severe Fuel Damage Research Partic-
c       ipation.  This Article limits the dissemination which can be made by
c       the receiving party.
C
        COMMON PERIM,AX,EMICEO,EMICE,AS2,AD2,XICE,PI,K,TOUT(100),
     1  TOG,TGAS,FMH2OI,FMVH2O,FMAIR,FMCO,FMCO2,FMH2,FILM
        DIMENSION TI(10),DPART(20),RHO(10),SOLF(10),PARCON(20,10)
     1  ,XH2I(10),XH2OI(10),TGASIN(10),PGASIN(10),XCOI(10),
     2  XAIRI(10),XCO2I(10),TGSOUT(10),XOH2OI(10),
     3  PMDOT(20),PRCON(20),DFOV(20),VSET(20),UPH2O(20)
```

```
     4  ,DFD(20),TG(2)
     5  ,AMD(20),AN(20),DPARTW(20),WPMDOT(20),GASINI(10),
     6  CHII(10),AKN(20),CMI(20),DFTH(20),DFNZ(20),DFNZ0(20)
     7  ,CLAMB(20),RDPAR(20),WRHO(20),WFWET(20),QUALI(10),
     8  BN(20),ET(2),XH(2),BK(20),PNDOT(20),D1(20),D2(20),
     9  WH2OT(20),WH2OUP(20),FN(20),OPMDOT(20),PMULT(20),DMULT(20)
        DIMENSION XARRAY(10),YARRAY(10)
C
C       DPART BELOW REPRESENT LOG NORMAL DISTRIBUTION ABOUT 1 MICRON
C
        DATA DPART/.076E-4,.1E-4,.13E-4,.17E-4,.22E-4,.3E-4,.39E-4,
     +  .52E-4,.68E-4,.84E-4,1.1E-4,1.5E-4,2.E-4,2.6E-4,3.5E-4,
     +  4.5E-4,5.9E-4,7.8E-4,9.5E-4,10.3E-4/
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C       ICEDF INPUT VARIABLES
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C       NDATA = 1,.........,50 MAX , NUMBER OF TIME POINTS FOR DATA ENTRY
C       TI(J),J=1,NDATA , TIME VALUES AT EACH NDATA (MINUTES)
C       DPART(I),I=1,.........,20 CHARACTERISTIC DIAMETER OF EACH OF 20
C                PARTICLE BUCKETS (CM)
C       RHO(J),J=1,NDATA  , PARTICLE DENSITY (G/CC)
C       SOLF(J),J=1.NDATA , WEIGHT FRACTION SOLUBLE MATERIAL
C       PARCON(I,J)       , PARTICLES IN EACH SIZE CLASS (G/CC)
C       XH2I(J)           , HYDROGEN MOLE FRACTION IN INLET GAS
```

```
C       XH2OI(J)          , WATER MOLE FRACTION IN INLET GAS
C       QUALI(J)          , QUALITY OF WATER IN INLET GAS (%)
C       TGASIN(J)         , INLET GAS TEMPERATURE (C)
C       PGASIN(J)         , INLET GAS ABSOLUTE PRESSURE (ATM)
C       XCOI(J)           , CARBON MONOXIDE MOLE FRACTION IN INLET GAS
C       XAIRI(J)          , AIR MOLE FRACTION IN INLET GAS
C       XCO2I(J)          , CARBON DIOXIDE MOLE FRACTION IN INLET GAS
C       TGSOUT(J)         , OUTLET GAS TEMPERATURE (C)
C       XOH2OI(J)         , MOLE FRACTION OF WATER IN OUTLET GAS
C       AS1I              , SEDIMENTATION AREA (CM**2)
C       AS2I              , SEDIMENTATION AREA (CM**2) FOR ICE
C       AS3I              , SEDIMENTATION AREA (CM**2)
C       AS4I              , SEDIMENTATION AREA (CM**2)
C       AI1I              , IMPACTION AREA (CM**2)
C       AI2I              , IMPACTION AREA (CM**2) FOR ICE
C       AD1I              , DIFFUSION AREA (CM**2)
C       AD2I              , DIFFUSION AREA (CM**2) FOR ICE
C       AD3I              , DIFFUSION AREA (CM**2)
C       AD4I              , DIFFUSION AREA (CM**2)
C       EFI               , ICE EFFICIENCY PARAMETER (DIMENSIONLESS)
C       GASINI(J),J=1,NDATA,GAS INLET FLOWRATE (M**3/SEC)
C       CHII(J),J=1,NDATA , SHAPE FACTOR FOR STOKES DRAG
C       KOUT=1,.....,100  , NUMBER OF OUTPUT STEPS
C       TOUT(K),K=1,....,KOUT  , SPECIFIED OUTPUT TIMES (MIN)
C       NZ = MAXIMUM INDEX OF VERTICAL ICE CALCULATIONAL ELEMENTS
C       CT = THERMAL ACCOMODATION CONSTANT
C       CMOM = MOMENTUM ACCOMODATION CONSTANT
C       VOLCON=CONTAINMENT VOLUME (CM**3)
C       MICE = 0 ICEMELT SUPRESSED
C
C
```

```
      AAP=3.2437814
      BP=5.868263E-03
      CP=1.17023793E-08
      DP=2.1878462E-03
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C     READ INPUT DATA
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
      OPEN(UNIT=4,NAME='ICEDF.DAT',TYPE='OLD',READONLY)
      READ(4,*)NDATA
      PRINT * , 'NDATA=',NDATA
      READ(4,*)(TI(I),I=1,NDATA)
      PRINT * , 'TI(I)=',(TI(I),I=1,NDATA)
      READ(4,*)(RHO(I),I=1,NDATA)
      PRINT * , 'RHO(I)=',(RHO(I),I=1,NDATA)
      READ(4,*)(SOLF(I),I=1,NDATA)
      PRINT * , 'SOLF(I)=',(SOLF(I),I=1,NDATA)
      DO 5 J=1,20
      READ(4,*)(PARCON(J,I),I=1,NDATA)
      PRINT * , 'PARCON(J,I)=',(PARCON(J,I),I=1,NDATA)
5     CONTINUE
      READ(4,*)(TGASIN(I),I=1,NDATA)
      PRINT * , 'TGASIN(I)=',(TGASIN(I),I=1,NDATA)
```

```
        READ(4,*)(PGASIN(I),I=1,NDATA)
        PRINT * , 'PGASIN(I)=',(PGASIN(I),I=1,NDATA)
        READ(4,*)(XH2I(I),I=1,NDATA)
        PRINT * , 'XH2I(I)=',(XH2I(I),I=1,NDATA)
        READ(4,*)(QUALI(I),I=1,NDATA)
        PRINT *,'QUALI(I)=',(QUALI(I),I=1,NDATA)
        READ(4,*)(XH2OI(I),I=1,NDATA)
        PRINT * , 'XH2OI(I)=',(XH2OI(I),I=1,NDATA)
        READ(4,*)(XOH2OI(I),I=1,NDATA)
        PRINT * , 'XOH2OI(I)=',(XOH2OI(I),I=1,NDATA)
        READ(4,*)(XCOI(I),I=1,NDATA)
        PRINT * , 'XCOI(I)=',(XCOI(I),I=1,NDATA)
        READ(4,*)(XCO2I(I),I=1,NDATA)
        PRINT * , 'XCO2I(I)=',(XCO2I(I),I=1,NDATA)
        READ(4,*)(XAIRI(I),I=1,NDATA)
        PRINT * , 'XAIRI(I)=',(XAIRI(I),I=1,NDATA)
        READ(4,*)(TGSOUT(I),I=1,NDATA)
        PRINT * , 'TGSOUT(I)=',(TGSOUT(I),I=1,NDATA)
        READ(4,*)(GASINI(I),I=1,NDATA)
        PRINT * , 'GASINI(I)=',(GASINI(I),I=1,NDATA)
        READ(4,*)(CHII(I),I=1,NDATA)
        PRINT * , 'CHII(I)=',(CHII(I),I=1,NDATA)
        READ(4,*)(PMULT(I),I=1,NDATA)
        PRINT * , ' PMULT(I)=',(PMULT(I),I=1,NDATA)
        READ(4,*)(DMULT(I),I=1,NDATA)
        PRINT * , ' DMULT(I)=',(DMULT(I),I=1,NDATA)
        READ(4,*)AS1,AS2,AS3,AS4,AI1,AI2,AD1,AD2,AD3,AD4
        PRINT * , ' AS1=',AS1,' AS2=',AS2,' AS3=',AS3,' AS4=',AS4
    1    ,' AI1=',AI1,' AI2=',AI2,' AD1=',AD1,' AD2=',AD2,' AD3=',AD3,
    2    ' AD4=',AD4
        READ(4,*)NZ,CT,CMOM,KOUT,VOLCON,MICE,XICE,EF
```

```
       PRINT * , ' NZ=',NZ,
     1 ' CT=',CT,' CMOM=',CMOM,' KOUT=',KOUT,' VOLCON=',VOLCON
     2 ,' MICE=',MICE,' XICE=',XICE,' EF=',EF
       READ(4,*)(TOUT(K),K=1,KOUT)
       PRINT * , 'TOUT(K)=',(TOUT(K),K=1,KOUT)
C      RG=82.06 (GAS CONSTANT IN CC ATM/GMOLE-K)
       RG=82.06
       PI=3.14159265
C
C      RH=HYDRAULIC RADIUS
C
C      AX=CM**2 PER UNIT XSXN BETWEEN 4 ICE BASKET COLUMNS
C
C      PERIM=CONTACT PERIMETER OF EACH FLOW COLUMN
C
C      NUNIT=NO. OF FLOW COLUMNS IN ICEBED
C
C      EMICE0 = INITIAL MASS OF ICE PER COLUMN (GRAMS)
C      XICE = FRACTION OF INITIAL MASS REMAINING
C
       NUNIT=1944
       DIA=30.48*SQRT(XICE)
       PERIM=PI*DIA
       AX=-PI*(DIA**2)/4.+1296.
       RH=AX/PERIM
       RH4=4.*RH
       EMICE0=5.144E+05
       EMICE=EMICE0*XICE
       FILM=0.
C
C      MASSAGE INPUT DATA
C
C      DETERMINE MOLE FRACTION OF NONCONDENSABLE GASES
C      AND ACTUAL VALUES AT TIME T
```

```
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C      MAJOR COMPUTATION LOOP (TO END OF PROGRAM)
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
      DO 1000 K=1,KOUT
      JOUT=NDATA-1
      DO 999 JM=1,JOUT
C
C      THIS LOOP ESTABLISHES INTERPOLATION VALUES
C
      IF(TOUT(K).GE.TI(JM).AND.TOUT(K).LT.TI(JM+1))JIN=JM
 999  CONTINUE
      DINT=(TOUT(K)-TI(JIN))/(TI(JIN+1)-TI(JIN))
      PMUL=PMULT(JIN)+DINT*(PMULT(JIN+1)-PMULT(JIN))
      DMUL=DMULT(JIN)+DINT*(DMULT(JIN+1)-DMULT(JIN))
      DO 998 JP=1,20
      PRCON(JP)=PARCON(JP,JIN)+DINT*(PARCON(JP,JIN+1)-PARCON(JP,JIN))
C
C      PARCON MULTIPLIER, PMULT
C
      PRCON(JP)=PRCON(JP)*PMUL
      DPART(JP)=DPART(JP)*DMUL
 998  CONTINUE
      XH2=XH2I(JIN)+DINT*(XH2I(JIN+1)-XH2I(JIN))
      XH2O=XH2OI(JIN)+DINT*(XH2OI(JIN+1)-XH2OI(JIN))
      XCO=XCOI(JIN)+DINT*(XCOI(JIN+1)-XCOI(JIN))
      XCO2=XCO2I(JIN)+DINT*(XCO2I(JIN+1)-XCOI(JIN))
      XAIR=XAIRI(JIN)+DINT*(XAIRI(JIN+1)-XAIRI(JIN))
      TGAS=TGASIN(JIN)+DINT*(TGASIN(JIN+1)-TGASIN(JIN))
```

```
      XOH2O=XOH2OI(JIN)+DINT*(XOH2OI(JIN+1)-XOH2OI(JIN))
      TGOUT=TGSOUT(JIN)+DINT*(TGSOUT(JIN+1)-TGSOUT(JIN))
      GASIN=GASINI(JIN)+DINT*(GASINI(JIN+1)-GASINI(JIN))
      CHI=CHII(JIN)+DINT*(CHII(JIN+1)-CHII(JIN))
      SOLFT=SOLF(JIN)+DINT*(SOLF(JIN+1)-SOLF(JIN))
      PGAS=PGASIN(JIN)+DINT*(PGASIN(JIN+1)-PGASIN(JIN))
      RHOT=RHO(JIN)+DINT*(RHO(JIN+1)-RHO(JIN))
      QUAL=QUALI(JIN)+DINT*(QUALI(JIN+1)-QUALI(JIN))
      GASIN=1.E+06*GASIN
C     GASIN IN CM**3/S
      UI=GASIN/AX/NUNIT
C     UI=SUPERFICIAL VELOCITY = IMPACTION VELOCITY (CM/S)
      AS1Z=AS1/NZ
      AS2Z=AS2*EF/NZ*XICE**.5
C
C     FOR IMPACTION
C
      AI1Z=AI1/NZ
C
C     FOR DIFFUSION
C
      AD1Z=AD1/NZ
      AD2Z=AD2*EF/NZ*XICE**.5
      AD3Z=AD3/NZ
      DZ=1460./NZ
C
      PS=0.
      DO 997 I=1,20
      PMDOT(I)=GASIN*PRCON(I)
      OPMDOT(I)=PMDOT(I)
      PS=PS+PMDOT(I)
      PNDOT(I)=PMDOT(I)/(RHOT*PI*DPART(I)**3./6.)
  997 CONTINUE
C
```

```
C     PS=TOTAL MASS FLOW RATE OF SOLIDS
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C     ESTABLISH INLET PARAMENTERS
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
      TIG=TGAS+273.2
      TG(1)=TIG
      TG(2)=TG(1)-(TGAS-TGOUT)/NZ
      XH(1)=XH2O
      XH(2)=XH(1)-(XH2O-XOH2O)/NZ
      AMW=2.*XH2+29.*XAIR+28.*XCO+44.*XCO2+18.*XH(1)
      RHOGAS=AMW*PGAS/(RG*TG(1))
C
C     WLDOT = MASS RATE OF LIQUID WATER ENTERING (GM/SEC)
C     WVDOT = MASS RATE OF WATER VAPOR ENTERING (GM/SEC)
C     TMDOT = TOTAL MOLAR GAS + VAPOR RATE ENTERING (GMOLES/S)
C
      TMDOT=GASIN*PGAS/(RG*TG(1))
      WVDOT=XH(1)*TMDOT*18.
      WLDOT=WVDOT*(100./QUAL-1.)
C
      RHOL=1.
      VAPL=4.5E+04
      CPH2=28.9
      CPLH2O=75.3
      CPVH2O=33.6
      CPCO=29.1
      CPCO2=37.2
      CPAIR=29.2
      CPMIX=CPH2*XH2+CPVH2O*XH(1)+CPCO*XCO+CPCO2*XCO2+CPAIR*XAIR
C
```

```
C     ALL CP'S IN J/GMOLE*K, VAPL IN J/GMOLE
C
      VLDOT=WLDOT/RHOL
      VSDOT=PS/RHOT
      GFLOW=GASIN
C
C     MOLAR FLOW RATES PER CHANNEL
C
      FMAIR=TMDOT*XAIR/NUNIT
      FMCO2=TMDOT*XCO2/NUNIT
      FMCO=TMDOT*XCO/NUNIT
      FMH2=TMDOT*XH2/NUNIT
      FMVH2O=XH2O*TMDOT/NUNIT
      FMLH2O=FMVH2O*WLDOT/WVDOT
      FMH2O=FMVH2O+FMLH2O
      FMGT=FMAIR+FMCO+FMCO2+FMH2+FMVH2O
C
C     DEFINE FMH2OI AS VAPOR INLET CONDITION FOR ICEMELT SUBROUTINE
C
      FMH2OI=FMVH2O
C
C     DEFINE ENERGY (ENTHALPY) FLOW AT CONTROL VOLUME (CV)
C     ENTRANCE ET(1) AND EXIT ET(2). BOTH IN J/S OR WATTS
C
      ET(1)=(FMH2*CPH2+FMCO*CPCO+FMCO2*CPCO2+FMAIR*CPAIR+FMLH2O*
     1 CPLH2O+FMVH2O*CPVH2O)*(TG(1)-273.2)+FMVH2O*VAPL
      XP1=647.27-TIG
      PV1=218.167*10.**(-(XP1/TIG)*(AAP+BP*XP1+CP*(XP1**3.))/(1.+DP*
     1 XP1))
C
C     SATN=AVERAGE SATURATION OF GAS IN ICEBED
C
      SATN=(XH2O/PV1)*PGAS
C
```

```
C       START PARTICLE GROWTH CALCULATIONS
C
C       GIVEN:
C       RHOT, DRY PARTICLE DENSITY OF DIAM=DPART(IP)
C       IF QUALITY LT 100%, BYPASS
        IF(QUAL.LT.100.)GO TO 4000
C
C       CALCULATE:
C       WET PARTICLE DIAM=DPART(IP)*RDPAR(IP)
C       AND CORRESPONDING DENSITY WRHO
C
        IF(SOLFT.GT.0.)GO TO 331
        RDPART=((VLDOT+VSDOT)/VSDOT)**0.3333
        WFWET1=WLDOT/(WLDOT+PS)
        WRHO1=(PS+WLDOT)/(VLDOT+VSDOT)
 331    IF(SOLFT.GT.0.)CALL SOLGRO(SATN,SOLFT,RHOT,WRHO1,WFWET1,RDPART)
 4000   CONTINUE
        DO 250 JP=1,20
        WRHO(JP)=WRHO1
        WFWET(JP)=WFWET1
        RDPAR(JP)=RDPART
        WH2OT(JP)=0.
 250    CONTINUE
C
C       FIRST STEP IS TO CALCULATE SETTLING AND DIFFUSION AT BOTTOM
C       OF ICE COMPARTMENT
C
        PS=0.
        CALL VISC(TG(1),XH(1),XH2,XCO,XAIR,XCO2,AMW1,VISMIX,AKG)
        DO 200 IP=1,20
        CALL DIFFU(DPART(IP),RDPAR(IP),VISMIX,TIG,AMW1,PGAS,DIFUS,CM,ELAM)
        CALL VSETL(WRHO(IP),CM,DPART(IP),RDPAR(IP),VISMIX,AMW1,PGAS,
     +  TG(1),RHOGAS,VSET(IP))
        DIFP=DIFUS
```

```
      IF(K.EQ.1..AND.XICE.GT.0.OR.XICE.GT.0..AND.MICE.EQ.0)TFILM=273.2
      IF(K.GT.1.AND.XICE.GT.0..AND.MICE.NE.0)GO TO 196
      GO TO 197
  196 HTO=HVSAVE+HCSAVE
      HSU=1./(1./HTO+FILM/.0056)
      TFILM=TG(1)*(1.-HSU/HTO)+273.2*HSU/HTO
  197 IF(XICE.EQ.0.)TFILM=TIG
      XP3=647.27-TFILM
      XPONEN=-(XP3/TFILM)*(AAP+BP*XP3+CP*(XP3**3.))/(1.+DP*XP3)
      PFILM=218.167*10.**XPONEN
      PFS=PFILM/PGAS

      DELT=(TIG-TFILM)
      IF(DELT.LT.0.OR.XICE.EQ.0.)DELT=0.
      IF(XICE.NE.0.)GO TO 198
      TG(1)=TIG
      TG(2)=TIG
  198 CONTINUE
      DTLM=DELT
      VISFLM=VISMIX
      CALL IID(CMI,CHI,RDPAR(IP),DPART(IP),VISMIX,VISFLM,UI,
     1 WRHO(IP),DIFP,RHOGAS,TG(1),DELT,RH4,AKG,AMW,CPMIX,AKD,
     2 EBD,EI,HV)
      AKS=VSET(IP)*AS3
      AKDB=AKD*2.*AS3
      RDPAR(IP)=RDPART
      DFOV(IP)=1.+(AKS+AKDB)/GASIN
      PMDOT(IP)=PMDOT(IP)/DFOV(IP)
      PNDOT(IP)=PNDOT(IP)/DFOV(IP)
      PS=PS+PMDOT(IP)
C
C     CONVERT PMDOT/PNDOT TO PER CHANNEL BASIS
C
      PMDOT(IP)=PMDOT(IP)/NUNIT
```

```
      PNDOT(IP)=PNDOT(IP)/NUNIT
      AN(IP)=PRCON(IP)*AX*DZ/DFOV(IP)
      IF(AN(IP).LE.1.E-20)AN(IP)=1.E-20
C
C     AN(IP) = NO. OF IP PARTICLES IN 1ST ICE SLAB DZ
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C     END OF ENTRANCE OF PER PARTICLE SIZE GROUP
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
200   CONTINUE
      VSDOT=PS/RHOT
      VLDOT=VSDOT*(RDPART**3.)-VSDOT
      WLDOT=VLDOT*RHOL
      S=SATN
      DXI=0.
      AKP=(1.-WFWET1)*.06+WFWET1*.0068
C
C     AKP = PARTICLE THERMAL CONDUCTIVITY, WATTS/CM/K
C
C     START MARCH ALONG ICEBED WITH NZ
C     FIRST ESTABLISH PARTICLE LOSS BASED ON INPUT CONDITIONS
C
      GFLOW=GASIN
      DELTT=TG(2)-TG(1)
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
      DO 290 MZ=1,NZ
      DELT=TG(1)-TFILM
      IF(DELT.LE.01)DELT=.01
      FH2O=0.
      TAV=(TG(1)+TFILM)/2.
```

```
      CALL VISC(TFILM,XH(1),XH2,XCO,XAIR,XCO2,AMW1,VISMIX,AKG)
      VISFLM=VISMIX
C
C     VISFLM=GAS VISCOSITY AT WALL
C
      CALL VISC(TG(1),XH(1),XH2,XCO,XAIR,XCO2,AMW1,VISMIX,AKG)
C     GO TO 605
      DO 201 IP=1,20
      CALL DIFFU(DPART(IP),RDPAR(IP),VISMIX,TG(1),AMW1,PGAS,DIFUS,CM,ELAM)
      CALL VSETL(WRHO(IP),CM,DPART(IP),RDPAR(IP),VISMIX,AMW1,PGAS,
     + TG(1),RHOGAS,VSET(IP))
      CALL IID(CMI,CHI,RDPAR(IP),DPART(IP),VISMIX,VISFLM,UI,
     1 WRHO(IP),DIFP,RHOGAS,TAV,DELT,RH4,AKG,AMW,CPMIX,AKD,
     2 EBD,EI,HV)
      AKS=VSET(IP)*(AS1Z+AS2Z)
      AKI=UI*AI1Z*EI
      AKDB=UI*AD1Z*EBD+AKD*(AD2Z+AD3Z)
      DFNZ(IP)=1.+(AKS+AKI+AKDB)/GFLOW
C
C     ADD THERMOPHORETIC TERM (DFTH(IP))
C
      AKN(IP)=ELAM*2./(DPART(IP)*RDPAR(IP))
      CTH=1.5*VISMIX*CM/(RHOGAS*TG(1))
      AKP=(1.-WFWET(IP))*.06+WFWET(IP)*.0068
      CTH=CTH*(AKG/AKP+CT*AKN(IP))
      CTH=CTH/(1.+3.*CMOM*AKN(IP))
      CTH=CTH/(1.*2.*AKG/AKP+2.*CT*AKN(IP))
      CMI(IP)=CM
      DFTH(IP)=1.-CTH*DELTT
C
C     ADD DIFFUSIOPHORETIC TERM (DFD)
C
      DFD(IP)=(1.-XH(2))/(1.-XH(1))
C
```

```
C     COMBINE ALL DF'S
C
      DFNZO(IP)=DFD(IP)*DFTH(IP)*DFNZ(IP)
      CLOG=ALOG10(DFNZO(IP))+ALOG10(DFOV(IP))
      IF(CLOG.GT.30.)GO TO 555
      DFOV(IP)=DFOV(IP)*DFNZO(IP)
      GO TO 402
555   DFOV(IP)=1.E+30
402   CONTINUE
C
C     RELATE DF TO MASS TRANSFER COEFF, BK(I) (CM/SEC)
C
      IF(PERIM.EQ.0.)GO TO 403
      BK(IP)=(UI*AX*(1.-1./DFNZO(IP)))/(DZ*PERIM)
403   CONTINUE
      IF(PERIM.EQ.0.)BK(IP)=0.
C
C     FLUX OF PARTICLES TO WALL, FN(IP) (GM/CM**2*SEC)
C
      FN(IP)=(BK(IP)*AN(IP)/(AX*DZ))*((DPART(IP)*RDPAR(IP))**3.-
     1 DPART(IP)**3.)*PI*RHOL/6.
      DOS=DPART(IP)*RDPAR(IP)
C
C     LOSS OF WATER TO ICE VIA PARTICLES, FH2O (GM/SEC)
C
      FH2O=FH2O+FN(IP)*PERIM*DZ
      AN(IP)=AN(IP)/DFNZO(IP)
      IF(AN(IP).LE.1.E-35)AN(IP)=1.E-35
      PNDOT(IP)=PNDOT(IP)/DFNZO(IP)
      IF(PNDOT(IP).LT.1.)PNDOT(IP)=1.
      PMDOT(IP)=PNDOT(IP)*RHOT*PI*(DPART(IP)**3.)/6.
      WRHO(IP)=(RHOL*(DOS**3.-DPART(IP)**3.)+RHOT*DPART(IP)**3)/
     1 DOS**3
      WFWET(IP)=RHOL*(DOS**3.-DPART(IP)**3.)/(RHOL*(DOS**3.-DPART(IP)
```

```
     1  **3.)+RHOT*DPART(IP)**3.)
201     CONTINUE
C
C       END PARTICLE LOSS CALCULATIONS
C
C
C       CALCULATE CONDENSATION HT. COEFF. USING UCHIDA CORRELATION
C
        WH=FMVH20*18.
        WA=FMAIR*29.+FMCO*28.+FMCO2*44.+FMH2*2.
        IF(WH/WA.LE.0.)GO TO 208
        HC=4.502E-02*(WH/WA)**.8
        IF(HC.GT..15889)HC=.15889
        AXH20=FMVH20/(FMAIR+FMVH20+FMCO+FMCO2+FMH2)
        IF(AXH20.LE.PFS)HC=0.
        GO TO 209
208     HC=0.
209     CONTINUE
C
C       ABOVE HC IN WATTS/CM**2*DEG K
C
C       CALCULATE PARTICLE GROWTH RATE CONSTANTS
C       FROM BYERS, P.112
        APR=EXP(13.5008-1.11063E-02*(TG(1)-273.2))
        BPR=EXP(13.7102-6.45E-02*(TG(1)-273.2))
        APP=APR*RHOL
        BPP=BPR*RHOL
C
C
C       COMPUTE DROPLET GROWTH
C
C
        SUMFL=0.
        IF(S.LT.1.AND.SOLFT.GT.0.)CALL SOLGRO(S,SOLFT,RHOT,WRHO1,
```

```
     1 WFWET1,RDPART)
C
C
      DO 1002 KP=1,20
      IF(S.GE.1.)GO TO 333
      RDPAR(KP)=RDPART
      WRHO(KP)=WRHO1
      WFWET(KP)=WFWET1
  333 CONTINUE
      IF(S.GT.1.)CALL KELVIN(TG(1),S,DPART(KP),RDPAR(KP),KP,NKLVN)
      D1(KP)=DPART(KP)*RDPAR(KP)
      EMP=(DPART(KP)**3.)*RHOT
      EMW=D1(KP)**3.-DPART(KP)**3.
      WFWET(KP)=EMW/(EMP+EMW)
 1002 CONTINUE
      DO 1001 JP=1,20
      IF(PNDOT(JP).LT.1.)PNDOT(JP)=1.
 1001 CONTINUE
      DO 202 IP=1,20
      IF(S.LT.1..OR.NKLVN.EQ.20)GO TO 303
      DENOM=0.
      TWAV=DXI*18.
C
C     TWAV=SUPERSATURATION WATER AVAILABLE FOR PARTICLE GROWTH,
      GRAMS/SEC/CHANNEL
C
      NK=NKLVN+1
      DO 2001 MP=NK,20
      DENOM=DENOM+PNDOT(MP)*D1(MP)
 2001 CONTINUE
      AMULT=TWAV/DENOM
      IF(IP.LE.NKLVN)AMULT=0.
      WH2OUP(IP)=AMULT*D1(IP)
      WH2OT(IP)=WH2OT(IP)+WH2OUP(IP)
```

```
      D2(IP)=(D1(IP)**3+6.*WH2OUP(IP)/(PI*RHOL))**0.33333
      GO TO 304
303   D2(IP)=D1(IP)
304   CONTINUE
      WH2OUP(IP)=PI*RHOL*(D2(IP}**3.-D1(IP)**3.)/6.
C
C     WH2OT(IP)=WATER (GRAMS) INCREASED PER DROP
C
      RDPAR(IP)=RDPAR(IP)*D2(IP)/D1(IP)
      WH2OT(IP)=PI*RHOL*(D2(IP)**3.-DPART(IP)**3.)/6.
      IF(S.LT.1.)WH2OT(IP)=0.
202   CONTINUE
C
C     WATER LOSSES TO WALL BY CONDENSATION
C
C     DEFINE WVWALL=GM/SEC WATER LOSS TO WALLS BY CONDENSATION
C
      WVWALL=HC*PERIM*DZ*(TG(1)-TFILM)/(VAPL/18.)
C
C     TOTAL WATER LOSS RATE (GM/SEC) = TWLR
C
      TWLR=WVWALL+FH2O
C
C     NEW FLOW OF WATER VAPOR OUT OF DZ, FMVH2O (GMOLES/SEC)
      FMLH2O=SUMFL/18.
      FMVH2O=FMH2O-(TWLR)/18.-FMLH2O
      FMGT3=FMH2+FMCO+FMCO2+FMAIR
      AFILM=PFS/(1.-PFS)
      IF(FMVH2O.LT.0.)GO TO 600
      GO TO 601
600   DELF=FMVH2O
      TWLR=TWLR-18.*DELF
      FMVH2O=AFILM*FMGT3
601   CONTINUE
```

```
      AMFH2O=FMVH2O/FMGT3
      A3X=FMVH2O
      IF(AMFH2O.LT.AFILM)FMVH2O=AFILM*FMGT3
      A4X=A3X/FMVH2O
      WVWALL=A4X*WVWALL
      HC=A4X*HC
C
C     NEW TOTAL FLOW OF WATER OUT OF DA, FMH2O
C
      FMH2O=FMLH2O+FMVH2O
C
C     HEAT BALANCE NEXT
C     SENSIBLE HEAT LOSS TO ICE, QSENS (WATTS) FROM GAS
C
C
C     CONDENSATION HEAT LOSS TO WALLS, QCOND (WATTS)
C
      QCOND=PERIM*DZ*HC*(TG(1)-273.2)
C
C     CORRECT HV FOR HIGH MASS TRANSFEF (BSL, p. 662)
C
      PHT=-HC/(HV+HC)
      IF(PHT.EQ.0.)GO TO 19
      RT=EXP(PHT)-1.
      THT=PHT/RT
      HV=THT*HV
19    CONTINUE
C
C     HEAT LOSS TO ICE VIA MASS OF PARTICLES REMOVED, QPART (WATTS)
C     NEGLECT SOLID MASS
C
      QPART=FH2O*CPLH2O*(TG(1)-273.2)
      QSENS=PERIM*DZ*HV*(TG(1)-273.2)

```

```
C     SUM HEAT LOSS TO ICE, QSUM
C
      QSUM=QSENS+QCOND+QPART
C
C     CORRECTION FOR FILM THICKNESS, FILM
      IF(K.EQ.1)GO TO 20
      HTOT=HC+HV+FH20*CPLH20
      IF(HTOT.EQ.0.)GO TO 20
      HSUM=1./(1./HTOT+FILM/.0056)
      QSUM=PERIM*DZ*HSUM*(TG(1)-273.2)
      TFILM=TG(1)*(1.-HSUM/HTOT)+273.2*HSUM/HTOT
C
C     TFILM = TEMPERATURE OF WATER SURFACE, K.
C
   20 CONTINUE
      XP3=647.27-TFILM
      XPONEN=-(XP3/TFILM)*(AAP+BP*XP3+CP*(XP3**3.))/(1.+DP*XP3)
      PFILM=218.167*10.**XPONEN
      PFS=PFILM/PGAS
C
C     NEW ENTHALPY FLOW INTO NEXT CV, ET(2)
C
      ET(2)=ET(1)-QSUM
C
C     CALCULATE CV OUTLET TEMPERATURE, TG(2)
C
      QFM=FMH2*CPH2+FMCO*CPCO+FMC02*CPC02+FMAIR*CPAIR+
    1 FMVH20*CPVH20+FMLH20*CPLH20
      QTEST=ET(2)-FMVH20*VAPL
      IF(QTEST.LT.0.)FMVH20=ET(2)/VAPL
      FMH20=FMLH20+FMVH20
      TG(2)=273.2+(ET(2)-FMVH20*VAPL)/QFM
      IF(QTEST.LT.0.)TG(2)=TFILM
      IF(TG(2).GE.TG(1))TG(2)=TG(1)+DELTT
```

```
      IF(TG(2).LT.TFILM)TG(2)=TFILM
C
C     CALCULATE SATURATION, S
C
      FMGT2=FMH2+FMCO+FMCO2+FMAIR+FMVH2O
C
C     CALCULATE GAS HEAT CAPACITY (CPMIX), JOULE/GMOLE/K
C
      CPMIX=QFM/FMGT2
      XH(2)=FMVH2O/FMGT2
      XH2=FMH2/FMGT2
      XAIR=FMAIR/FMGT2
      XCO=FMCO/FMGT2
      XCO2=FMCO2/FMGT2
      XP3=647.27-TG(2)
      XPONEN=-(XP3/TG(2))*(AAP+BP*XP3+CP*(XP3**3.))/(1.+DP*XP3)
      PV3=218.167*10.**XPONEN
      XS=PV3/PGAS
      S=XH(2)/XS
      IF(S.LT.1.)GO TO 203
C
C     THIS NEXT SXN ADJUSTS TG(2) TO REFLECT THE FORMATION
C     OF CONDENSED H2O ON PARTICLES WHEN S.GE.1.
C
      TG1=TG(1)
      TG2=TG(2)
C     DO 205 MP=1,3
      TEMP=ABS(TG2-TG1)
      IF(TEMP.LT.0.001)TG2=TG1-.001
      DX1A=ET(2)-(TG1-273.2)*QFM-FMVH2O*VAPL
      DX1A=DX1A/((TG1-273.2)*(CPLH2O-CPVH2O)-VAPL)
      DX1B=ET(2)-(TG2-273.2)*QFM-FMVH2O*VAPL
      DX1B=DX1B/((TG2-273.2)*(CPLH2O-CPVH2O)-VAPL)
      X2A=647.27-TG1
```

```
      XPONEN=-(X2A/TG1)*(AAP+BP*X2A+CP*(X2A**3.))/(1.+DP*X2A)
      P2A=218.167*10.**XPONEN
      X2B=647.27-TG2
      XPONEN=-(X2B/TG2)*(AAP+BP*X2B+CP*(X2B**3.))/(1.+DP*X2B)
      P2B=218.167*10.**XPONEN
      DX2A=(PGAS*FMVH2O-P2A*FMGT2)/(PGAS-P2A)
      DX2B=(PGAS*FMVH2O-P2B*FMGT2)/(PGAS-P2B)
C
C     INTERSECT LINES DXI=AX2+BX2*TGI AND DXI=AX1+BX1*TGI
C
      BX1=(DX1A-DX1B)/(TG1-TG2)
      AX1=DX1A-BX1*TG1
      BX2=(DX2A-DX2B)/(TG1-TG2)
      AX2=DX2A-BX2*TG1
      TGI=(AX2-AX1)/(BX1-BX2)
      DXI=AX2+BX2*TGI
      TG(2)=TGI
      IF(DXI.LT.0.)DXI=0.
      IF(DXI.EQ.0.)S=1.
C
C     THIS SXN CALCULATES PARTICLE GROWTH WHEN FEWER PARTICLES EXIST
C
      S2=S
      IF(S2.GT.4.)S2=4.
      DTIME=DZ/UI
      TUPH2O=0.
      DO 206 IP=1,20
      DUP=0.
C     IF(IP.GT.NKLVN)
      DUP=2.*(S2-1.)*DTIME/(RHOL*(APP+BPP))
      RO=DPART(IP)*RDPAR(IP)/2.
      UPH2O(IP)=(RHOL*4.*PI/3.)*((RO**2.+DUP)**1.5-RO**3.)
C
C     UPH2O(IP)=MASS UPTAKE OF SINGLE IP PARTICLE IN DZ
```

```
C
      TUPH2O=UPH2O(IP)*PNDOT(IP)+TUPH2O
  206 CONTINUE
      OSTRU1=OSTRUE
      IF(OSTRU1.EQ.0.)OSTRU1=.0001
      DXS=TUPH2O/18.
      IF(DXI.GE.DXS)GO TO 12
      IF(DXI.EQ.0.)STRUE=1.
      IF(DXI.EQ.0..OR.DXS.EQ.0.)GO TO 13
      S3=DXS/DXI
      S4=S-1.
      STRUE=1.+S4/S3
      GO TO 13
   12 STRUE=S
   13 CONTINUE
      OSTRUE=STRUE-1.
      OSTRUE=SQRT(OSTRU1*OSTRUE)
      STRUE=1.+OSTRUE
      IF(DXS.GE.DXI)GO TO 203
      DXI=DXS
      TG(2)=273.2+(ET(2)+(-FMVH2O+DXI)*VAPL)/((CPLH2O-CPVH2O)*DXI+QFM)
  203 CONTINUE
      IF(S.LE.1.)TG(2)=273.2+ET(2)-FMVH2O*VAPL
      IF(DELTT.EQ.0.)DELTT=-.001
      IF(TG(2).GE.TG(1))TG(2)=TG(1)+DELTT
      IF(TG(2).LT.TFILM)TG(2)=TFILM
      DELTT=TG(2)-TG(1)
C
C     CONDENSATION RATE ON PARTICLES IS DXI, GMOLES/HR
C
C
C     CALCULATE NEW VELOCITY, UI
C
      UI=UI*FMGT2*TG(2)/(FMGT*TG(1))
```

```
C
C     NEW GAS DENSITY (RHOGAS) AVERAGE MOLECULAR WEIGHT
C
      AMW=(FMVH2O*18.+FMH2*2.+FMCO*28.+FMCO2*44.+FMAIR*29.)/FMGT2
      RHOGAS=AMW*PGAS/(RG*TG(2))
C
C     NEW GAS FLOW, GFLOW
      GFLOW=GFLOW*FMGT2*TG(2)/(FMGT*TG(1))
C     DTLM = LN MEAN TEMPERATURE DIRRERENCE
C     IF(TG(2).LE.TFILM)TG(2)=TFILM+.001
C     IF(TG(1).LE.TG(2))TG(1)=TG(2)+.001
C     DTLM=(TG(1)-TG(2))/ALOG((TG(1)-TFILM)/(TG(2)-TFILM))
C     IF(DTLM.LE..01)DTLM=.01
      DTLM=DELT
C
C     RETURN OF VARIABLES FOR NEXT MZ
C
      TG(1)=TG(2)
      DELH=XH(2)-XH(1)
      XH(1)=XH(2)
      XH(2)=XH(1)+DELH
      ET(1)=ET(2)
      FMGT=FMGT2
      IF(MZ.GT.1)GO TO 290
      HCSAVE=HC
      HVSAVE=HV
  290 CONTINUE
C
C     COMPUTE DF FOR NZ+1 SPCE
C
      CALL VISC(TG(1),XH(1),XH2,XCO,XAIR,XCO2,AMW1,VISMIX,AKG)
      DO 210 KP=1,20
      CALL DIFFU(DPART(KP),RDPAR(KP),VISMIX,TG(1),AMW1,PGAS,DIFUS,
     1 CM,ELAM)
```

```
      CALL VSETL(WRHO(KP),CM,DPART(KP),RDPAR(KP),VISMIX,AMW1,PGAS,
     + TG(1),RHOGAS,VSET(KP))
      DIFP=DIFUS
      CALL IID(CMI,CHI,RDPAR(KP),DPART(KP),VISMIX,VISFLM,UI,
     1 WRHO(KP),DIFP,RHOGAS,TG(1),DELT,RH4,AKG,AMW,CPMIX,AKD,
     2 EBD,EI,HV)
      AKDB=AKD*AD4
      AKS=VSET(KP)*AS4
      DFLAST=1.+(AKS+AKDB)/GFLOW
      BLOG=ALOG10(DFLAST)+ALOG10(DFOV(KP))
      IF(BLOG.GT.30.)GO TO 556
      DFOV(KP)=DFOV(KP)*DFLAST
      GO TO 557
  556 DFOV(KP)=1.E+30
  557 CONTINUE
      PMDOT(KP)=PMDOT(KP)/DFLAST
      PNDOT(KP)=PNDOT(KP)/DFLAST
C
C     CONVERT PMDOT/PNDOT BACK TO TOTAL FLOW BASIS
C
      PNDOT(KP)=PNDOT(KP)*NUNIT
      PMDOT(KP)=PMDOT(KP)*NUNIT
      AN(KP)=AN(KP)/DFLAST
      IF(AN(KP).LE.1.E-35)AN(KP)=1.E-35
      CLAMB(KP)=GASIN*(1.-1./DFOV(KP))/VOLCON
  210 CONTINUE
C
C
C     END OF CALCULATIONS
C
C     PREPARE OUTPUT INFORMATION
C
C     FLOWRATE OF DRY PARTICLE SIZE EXITING, (PMDOT(I)) AND
C     WET(WPMDOT(I)) AND TOTAL FLOWRATE OF PARTICLES (TFPO/TPFI)
```

```
      TOG=TG(2)-273.2
      TFPI=0.
      TFPO=0.
      WTFPO=0.
      TM=0.
      TV=0.
      DO 310 I=1,20
      IF(WFWET(I).GT..999)WFWET(I)=.999
      WPMDOT(I)=PMDOT(I)/(1.-WFWET(I))
      TFPI=TFPI+OPMDOT(I)
      TFPO=TFPO+PMDOT(I)
      WTFPO=WTFPO+PMDOT(I)/(1.-WFWET(I))
      TM=TM+WPMDOT(I)
      TV=TV+PMDOT(I)/RHOT+(WPMDOT(I)-PMDOT(I))/RHOL
  310 CONTINUE
      DFAP=TFPI/TFPO
      DLAMB=GASIN*(1.-1./DFAP)/VCLCON
      RHOW=TM/TV
      FWET=1.-TFPO/WTFPO
C
C     WTFPO = TOTAL FLOWRATE OF WET PARTICLES OUT OF ICE COLUMN
C
C     OUTPUT PARTICLE NUMBERS/SEC = AN(N)
C     MASS OF DRY PARTICLE, AMD(N)
C
      ANT=0.
      DO 311 I=1,20
      AMD(I)=RHOT*PI*(DPART(I)**3.)/6.
      BN(I)=PMDOT(I)/AMD(I)
C
C     ANT = TOTAL NUMBER FLOWRATE OF LEAVING PARTICLES
C
      ANT=ANT+BN(I)
  311 CONTINUE
```

```
C
C     ANMEND = NO. MEAN PARTICLE DIAM: DRY
C     ANMENW = NO. MEAN PARTICLE DIAM: WET
C     ANMEDD = NO. MEDIAN PARTICLE DIAM: DRY
C     ANMEDW = NO. MEDIAN PARTICLE DIAM: WET
      ANMEND=0.
      ANMENW=0.
      ANMEDD=0.
      ANMEDW=0.
      DO 312 I=1,20
      DPARTW(I)=DPART(I)*RDPAR(I)
      ANMEDD=ANMEDD+BN(I)*ALOG(DPART(I))
      ANMEDW=ANMEDW+BN(I)*ALOG(DPARTW(I))
      ANMEND=ANMEND+BN(I)*DPART(I)
      ANMENW=ANMENW+BN(I)*DPART(I)*RDPAR(I)
  312 CONTINUE
      ANMEDW=EXP(ANMEDW/ANT)
      ANMEDD=EXP(ANMEDD/ANT)
      ANMEND=ANMEND/ANT
      ANMENW=ANMENW/ANT
C
C     CALCULATE:
C     SIGWET = GEOMETRIC STD DEVIATION OF WET PARTICLES
C     SIGDRY = GEOMETRIC STD DEVIATION OF DRY PARTICLES
C
      SWET=0.
      SDRY=0.
      DO 313 N=1,20
      SWET=SWET+BN(N)*((ALOG(DPARTW(N)/ANMENW))**2.)
      SDRY=SDRY+BN(N)*((ALOG(DPART(N)/ANMEND))**2.)
  313 CONTINUE
      SIGWET=EXP((SWET/ANT)**.5)
      SIGDRY=EXP((SDRY/ANT)**.5)
      RADDRY=ANMEDD/2.
```

```
       RADWET=ANMEDW/2.
       RELH=S*100.
       WRITE(6,100)K,TOUT(K)
       DO 10 I=1,20
       WRITE(6,101)I,DPART(I),DPARTW(I),PMDOT(I),WPMDOT(I),BN(I),
     1 DFOV(I),CLAMB(I)
10     CONTINUE
       WRITE(6,104)RHOT,RHOW,FWET,RADDRY,RADWET,SIGDRY,SIGWET,TFPI,
     1 TFPO,DFAP,WTFPO,RELH,TOG,DLAMB,XICE
       DO 11 KP=1,20
       DPART(KP)=DPART(KP)/DMUL
11     CONTINUE
       IF(KOUT.GT.1.AND.K.LT.KOUT.AND.MICE.NE.0.AND.XICE.GT.0.)
     1 CALL ICEMELT
1000   CONTINUE
100    FORMAT(1H1,///,
     1 ' TOUT(',I3.3,')=',F7.2,' MINUTES. MATERIALS LEAVING',
     2 ' ICEBED',///,' PARTICLE',T12,'PARTICLE',T24,'PARTICLE',T37,
     3 'GRAMS',T49,'GRAMS',T60,'NUMBER',T72,'DECON.',T84,'LAMBDA',/,
     4 '   BIN',T13,'DIAM',T25,'DIAM',T36,'PER SEC',T48,'PER SEC',T60,
     5 'PER SEC',T72,'FACTOR',T84,'1/SEC',/,' NUMBER',T12,'DRY (CM)',
     6 T24,'WET (CM)',T37,'DRY',T49,'WET',T75,'DF',/)
101    FORMAT(1H T3,I2,T12,7(E10.4,2X))
104    FORMAT(1H0,//,T12,E10.4,T24,'DRY PARTICLE DENSITY (GM/CM**3)',/,
     1 T12,E10.4,T24,'WET PARTICLE DENSITY (GM/CM**3)',/,
     2 T12,E10.4,T24,'WEIGHT FRACTION WATER IN PARTICLES',/,T12,E10.4,
     3 T24,'NUMBER MEDIAN PARTICLE RADIUS OF DRY PARTICLES (CM)'
     4 ,/,T12,E10.4,
     5 T24,'NUMBER MEDIAN PARTICLE RADIUS OF WET PARTICLES(CM)'
     6 ,/,T12,E10.4,T24,'GEOMETRIC STANDARD DEVIATION OF DRY PARTICLES',
     7 /,T12,E10.4,T24,'GEOMETRIC STANDARD DEVIATION OF WET PARTICLES',
     8 /,T12,E10.4,T24,'TOTAL GRAMS/SEC DRY PARTICLES INTO ICEBED',/,
     9 T12,E10.4,T24,'TOTAL GRAMS/SEC DRY PARTICLES LEAVING ICEBED',/,
     1 T12,E10.4,T24,'INTEGRATED DECONTAMINATION FACTOR',/,
```

```
     2 T12,E10.4,T24,'TOTAL GRAMS/SEC WET PARTICLES LEAVING ICEBED',/,
     3 T12,E10.4,T24,'RELATIVE HUMIDITY OF GAS LEAVING ICEBED (PERCENT)'
     4 ,/,T12,E10.4,T24,'OUTLET GAS TEMPERATURE (DEG C)'
     5 ,/,T12,E10.4,T24,'REMOVAL LAMBDA FOR ALL PARTICLES (1/SEC)'
     6 ,/,T12,E10.4,T24,'FRACTION OF INITIAL ICE REMAINING')
       STOP
       END
       SUBROUTINE KELVIN(T,ST,DP,RD,K,N)
C
C      THIS SUBROUTINE DETERMINES IF PARTICLES CAN GROW UNDER
C      RESTRICTIONS OF KELVIN EQUATION FOR CURVED SURFACES.
C      GAMMA=SURFACE TENSION, ERG/CM**2
C
       TC=T-273.2
       GAMMA=66.2-(TC-60.)*0.1825
       IF(TC.LT.60.)GAMMA=75.7-.1583*TC
       V=18.
       R=DP*RD/2.
       RG=8.3136E+07
       PK=EXP(2.*GAMMA*V/(R*RG*T))
       N=0
       IF(PK.GT.ST)RD=1.
       IF(PK.GT.ST)N=K
C
C      SEE ADAMSON,A.W., PHYSICAL CHEMISTRY OF SURFACES, 3RD ED.,
C      WILEY,NY,1976.
C
       RETURN
       END
       SUBROUTINE DIFFU(DPART,RDPART,VISMIX,TAV,AMW,PGAS,DIFUS,CM,ELAM)
C
C      THIS SUBROUTINE CALCULATES PARTICLE DIFFUSIVITY, DIF(N)
C      AS A FUNCTION OF PARTICLE SIZE
C
```

```
C     INPUTS:
C     DPART, RDPART, VISMIX, TAV, AMW, PGAS
C
C     CUNNINGHAM FACTOR, CM AND ELAM, MEAN FREE PATH OF GAS
C
      PI=3.14159265
      ELAM=1.245E-02*((TAV/AMW)**.5)*VISMIX/PGAS
      DPA=DPART*RDPART
      IF(DPA.LT.1.E+3)GO TO 95
      RATD=ELAM/DPA
      CM=1.+2.492*RATD+0.84*RATD*EXP(-0.435/RATD)
      GO TO 90
   95 CM=1.
   90 CONTINUE
      DIFUS=1.38E-16*TAV*CM/(3.*PI*VISMIX*DPA)
C
C     OUTPUT: DIFFUSIVITY,DIFUS IN CM**2/SEC
C
      RETURN
      END
      SUBROUTINE VISC(TB,XAH2O,XH2,XCO,XAIR,XCO2,AMW,VISMIX,AKG)
      DIMENSION Y(5),VS(5),WM(5),Z(5),PHI(5,5),VK(5)
      SQRTTB=SQRT(TB)
      EPSH2O=809.1
      EPSH2=38.
      EPSAIR=97.
      EPSCO=110.
      EPSCO2=190.
      SIGH2O=2.641
      SIGH2=2.915
      SIGAIR=3.617
      SIGCO=3.59
      SIGCO2=3.996
C
```

```
C       DEFINE MOLE FRACTIONS WITH STEAM AMF2 MOLE FRACTION
C
        YH2O=XAH2O
        YH2=XH2
        YCO=XCO
        YCO2=XCO2
        YAIR=XAIR
        AMW=YAIR*29.+YCO2*44.+YCO*28.+YH2O*18.
        OMH2O=0.765+0.82*EPSH2O/TB
        VISH2O=2.6693E-05*SQRT(18.*TB)/((SIGH2O**2.)*OMH2O)
        OMH2=0.765+0.82*EPSH2/TB
        OMCO=0.765+0.82*EPSCO/TB
        OMCO2=0.765+0.82*EPSCO2/TB
        OMAIR=0.765+0.82*EPSAIR/TB
        VISH2=2.6693E-05*SQRT(2.*TB)/((SIGH2**2.)*OMH2)
        VISCO=2.6693E-05*SQRT(28.*TB)/((SIGCO**2.)*OMCO)
        VISCO2=2.6693E-05*SQRT(44.*TB)/((SIGCO2**2.)*OMCO2)
        VISAIR=2.6693E-05*SQRT(29.*TB)/((SIGAIR**2.)*OMAIR)
        AKGH2O=(.3268*SQRTTB-3.9179)/10000.
        AKGH2=(.1718*SQRTTB-1.15520)/10000.
        AKGCO=(.2583*SQRTTB-1.9407)/10000.
        AKGCO2=(.2795*SQRTTB-3.1296)/10000.
        AKGAIR=(.2716*SQRTTB-2.0671)/10000.
C       AKG - IN WATTS/CM/K
        Y(1)=YH2O
        Y(2)=YH2
        Y(3)=YCO
        Y(4)=YCO2
        Y(5)=YAIR
        VS(1)=VISH2O
        VS(2)=VISH2
        VS(3)=VISCO
        VS(4)=VISCO2
        VS(5)=VISAIR
```

```
      VK(1)=AKGH2O
      VK(2)=AKGH2
      VK(3)=AKGCO
      VK(4)=AKGCO2
      VK(5)=AKGAIR
      WM(1)=18.
      WM(2)=2.
      WM(3)=28.
      WM(4)=44.
```

```
          WM(5)=29.
          DO 301 J=1,5
          DO 301 I=1,5
          PHI(I,J)=1./(((1.+WM(I)/WM(J))*8.)**.5)*(1.+SQRT(VS(I)/VS(J))
        1 *(WM(J)/WM(I))**.25)**2
  301     CONTINUE
          DO 302 I=1,5
          Z(I)=0.
          DO 302 J=1,5
          Z(I)=Z(I)+Y(J)*PHI(I,J)
  302     CONTINUE
          AKG=0.
          VISMIX=0.
          DO 303 I=1,5
          VISMIX=VISMIX+Y(I)*VS(I)/Z(I)
          AKG=AKG+Y(I)*VK(I)/Z(I)
  303     CONTINUE
C
C         VISMIX IN POISES. CALCULATIONS USE BSL PAGE 24
C
          RETURN
          END
          SUBROUTINE VSETL(WRHO,CM,DPART,RDPAR,VISMIX,AMW,PGAS,TAV,
        1 RHOGAS,VSET1)
C         CALCULATE SETTLING VELOCITIES NOW (VSET1)
          G=980.
          RG=82.06
          VSET1=WRHO*G*CM*(DPART*RDPAR)**2./(18.*VISMIX)
C
C         FOLLOWING TAKEN FROM BNWL-1326, PAGE 12-13
C
```

```
      RHOGAS=AMW*PGAS/(RG*TAV)
      FDRE2=1.3333*WRHO*RHOGAS*G*((RDPAR*DPART)**3.)/(VISMIX**2.)
      IF(FDRE2.GT.9.6.AND.FDRE2.LT.93.6)RE=(FDRE2/27.)**(1./1.13)
      IF(FDRE2.GE.93.6.AND.FDRE2.LT.410.)RE=(FDRE2/24.32)**(1./1.227)
      IF(FDRE2.GE.410..AND.FDRE2.LT.1.07E+04)RE=(FDRE2/15.71)**
     1 (1./1.417)
      IF(FDRE2.GE.1.07E+04.AND.FDRE2.LT.2.45E+05)RE=(FDRE2/6.477)
     1 **(1./1.609)
      IF(FDRE2.GE.2.45E+05)RE=(FDRE2/1.194)**(1./1.867)
      IF(FDRE2.GT.9.6)VSET1=RE*VISMIX/(DPART*RDPAR*RHOGAS)
C
      RETURN
      END
      SUBROUTINE IID(CMI,CHI,RDPART,DPART,VISMIX,VISFLM,UI
     1 ,WRHO,DIFP,RHOGAS,TAV,DELT,RH4,AKG,AMW,CPMIX,AKD,EBD,EI,HV)
C
C     STOKES NUMBER (STK)
C
C     DC=COLLECTOR DIAMETER (CM)
C
      DC=.199
      STK=UI*WRHO*CMI*(RDPART*DPART)**2./(9.*VISMIX*
     1 DC*CHI)
C
C     IMPACTION EFFICIENCY (EIMP)
C
      EIMP=(STK/(STK+.5))*2.-.04
      IF(EIMP.LT.0.)EIMP=0.
C
C     INTERCEPTION EFFICIENCY (EINT)
C
      EINT=2.*RDPART*DPART/DC
C
C     OVERALL EFFICIENCY (EI)
```

```
      EI=EINT+EIMP
C
C     DIFFUSION COLLECTION PARAMETERS
C     PECLET NUMBER (PE)
C     DCD=DIFFUSION COLLECTOR DIAMETER
C
      DCD=.526
      PE=DCD*UI/DIFP
C
C     COLLECTOR REYNOLDS NUMBER (REDI)
C
      REDI=RHOGAS*DCD*UI/VISMIX
C
C     DIFFUSION EFFICIENCY (EBD)
C
      EBD=1./PE+1.727*(REDI**(1./6.))/(PE**(2./3.))
C
C     GRASHOF NUMBER DIVIDED BY L**3 (GRL)
C
      GRL=(980./(VISMIX/RHOGAS)**2.)*DELT/TAV
C
C     SCHMIDT NUMBER (SCH)
C
      SCH=VISMIX/(RHOGAS*DIFP)
C
C     DIFFUSION MASS XFER COEFF (AKD)
C
      AKD=DIFP*.13*(GRL*SCH)**(1./3.)
      IF(DELT.GT.0.)GO TO 5
      HV=0.
      RETURN
    5 CONTINUE
C
C     CONVECTIVE HT COEFF (HV),WATTS/CM**2/K
```

```
C
C        PRANDTL NUMBER, PR
```

```
      PR=VISMIX*CPMIX/AKG/AMW
C
C     HVF = FREE CONVECTION HT COEFF
C
      HVF=AKG*.13*(GRL*PR)**(1./3.)
C     FORCED CONVECTION HT COEFF FROM FIG. 13.2-1, BSL PAGE
C     400 FOR L/D=60.
C
C     RE = CHANNEL FLOW REYNOLDS NUMBER
C
      RE=RH4*RHOGAS*UI/VISMIX
      VIS=VISMIX/VISFLM
      IF(RE.LT.2100.)HV=(AKG/RH4)*(VIS**0.14)*0.475*(RE*PR)**.3333
      F1=RE*(PR**.3333)*(VIS**0.14)
      F2=10.**(-0.8715*(ALOG10(RE))**2.+6.49428*ALOG10(RE)-14.5052)
      F3=0.004
      F4=10.**(-0.192645*ALOG10(RE)-1.62736)
      IF(2100..LE.RE.AND.RE.LT.6000.)HV=F1*F2*AKG/RH4
      IF(6000..LE.RE.AND.RE.LT.10000.)HV=F1*F3*AKG/RH4
      IF(10000..LE.RE.AND.RE.LT.20000.)HV=F1*F4*AKG/RH4
      IF(RE.GE.20000.)HV=0.026*(AKG/RH4)*(RE**0.8)*(PR**0.3333)
     1 *(VIS**0.14)
      IF(HV.LT.HVF)HV=HVF
      RETURN
      END
      SUBROUTINE SOLGRO(SATN,SOLFT,RHOT,WRHO1,WFWET1,RDPART)
      PI=3.14159265
C
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
```

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C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C      THIS SUBROUTINE CALCULATES PARTICLE GROWTH DUE TO PARTICLE SOLUBILITY
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C<><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
C
C      PICK DPART=1 CM
C      WMC=MASS OF SOLUTE (AS CSOH)
       WMC=SOLFT*RHOT*PI/6.
C
C      WMS=MASS OF SOLVENT H20
C      WFWET=FRACTION OF MASS AS H20
C
       IF(SATN.GE..99)SATN=.99
       WMS=0.24*WMC/(1./SATN-1.)
       VI=(1.-SOLFT)*PI/6.
       RHOS=1.
       IF(WMC.EQ.0.)GO TO 332
       RHOS=1.+1.04*WMC/(WMC+WMS)
  332  VS1=(WMC+WMS)/RHOS
       WMI=RHOT*PI/6.
       WRHO1=(WMS+WMI)/(VI+VS1)
       RDPART=(6.*(VS1+VI)/PI)**.3333
       WFWET1=WMS/(WMI+WMS)
       RETURN
       END
       SUBROUTINE ICEMELT
C
C      THIS SUBROUTINE CALCULATES SOME OF THE PARAMETERS THAT CHANGE
C      AND THE WATER FILM THICKNESS AS THE ICE MELTS. THESE PARAMETERS
C      ARE PERIM,AX,AS2,AD2,XICE, AND FILM.
       COMMON PERIM,AX,EMICEO,EMICE,AS2,AD2,XICE,PI,K,TOUT(100),
```

```
     1 TOG,TGAS,FMH2OI,FMVH2O,FMAIR,FMCO,FMCO2,FMH2,FILM
C
C     ESTABLISH TIME STEP DT (SECONDS)
C
      DT=TOUT(K+1)-TOUT(K)
      DT=DT*60.
      EICE=EMICE
      EMSI=FMH2OI*18.
      EMSO=FMVH2O*18.
      DTMP=TGAS-TOG
      A=DTMP*(28.9*FMH2+29.1*FMCO+37.2*FMCO2+29.2*FMAIR)
      B=EMSI*(-2.4434*TGAS+2501.4)
      C=EMSO*(-(1.747*TOG+2501.4)+4.1904*TGAS)
      D=4.1904*TGAS+334.7
      DICE=-(A+B+C)*DT/D
      EMICE=EICE+DICE
      IF(EMICE.LT.0.)EMICE=0.
      DICE=EMICE-EICE
      XICE=EMICE/EMICE0
      DIA=SQRT(XICE*929.)
      PERIM=PI*DIA
      AX=1296.-PI*(DIA**2.)/4.
      AS2=AS2*DIA/30.48
      AD2=AD2*DIA/30.48
C
C     THE FOLLOWING ESTIMATES WATER FILM THICKNESS, FILM (CM),ON ICE.
C     W=WATER FLOW RATE (CC/S)
C
      W=EMSI-EMSO-DICE/DT
      IF(PERIM.EQ.0.)GO TO 2
      FILM=3.73E-02*(W/PERIM)**.3333
C
C     ABOVE FILM EQN=EQN 2.2-20, BSL AT 0 DEG C
C
```

```
      RETURN
    2 FILM=0.
      RETURN
      END
```

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This report describes the technical bases and use of computer code ICEDF. ICEDF was developed to serve as a tool for calculating particle retention in pressurized water reactor (PWR) ice compartments during severe accidents. This report also serves as a complete user's guide for the most recent stand-alone version of ICEDF. A complete code description, code operating instructions, code listing, examples of the use of ICEDF, and a summary of a parameter sensitivity study support the use of code ICEDF.

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