CHEMCON User's Manual

Version 3.1

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ABSTRACT

CHEMCON is a computer program developed to analyze thermal transients of tokamak fusion reactors. It contains a one dimensional, cylindrical geometry, conduction model that allows a variety of heat transfer modes within nodes and at node boundaries. Solid regions can be grouped into segments that communicate at their boundaries through a radiation enclosure model. CHEMCON includes a single volume, pressurization/condensation model that is used to include the effects of an in-vessel LOCA and the resulting heat transfer between hot surfaces and cold surfaces in contact with this volume. The code includes properties for 11 solid materials and two gases. CHEMCON also contains specialized models for modeling chemical reactions of node boundaries with air and steam including the gases produced from these reactions. In addition, a model treating the collapse of radiation shields within a gap is also included. CHEMCON is used mainly to simulate the thermal transient for post-blowdown loss-of-coolant-accidents.

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CHEMCON User's Manual

This document describes a thermal model that was developed for the International Thermonuclear Experimental Reactor (ITER) project to analyze long-term loss-of-cooling accidents. The following sections discuss the heat conduction equation, thermal modeling assumptions, material properties, and input requirements for the CHEMCON code. Section 1 presents the conduction equations used in the CHEMCON code and the pressurization/condensation model. Section 2 describes the oxidation reactions for steam and air with beryllium, graphite, and tungsten used in the CHEMCON code. Section 3 describes the material property relationships used in CHEMCON. Section 4 describes the philosophy behind the formulation of an input model for CHEMCON and gives a detailed description of the input format. Section 5 contains a list of References. Finally, Appendix A contains a summary of code testing, Appendix B contains the air and steam property tables and Appendix C includes a complete input model.

1. CONDUCTION EQUATION

The following one-dimensional cylindrical heat conduction equation was used in the CHEMCON code:¹

$$\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{d}{dr} \left(r k \frac{dT}{dr} \right) + q \quad (1)$$

where

- ρ = density (kg/m³)
- C_p = specific heat (J/kg · K)
- T = temperature (K)
- t = time (s)
- r = spatial variable (m)
- k = thermal conductivity (W/m · K)
- q = volumetric energy generation rate (W/m³).

Figure 1 shows a schematic of the boundaries of the "ith" computational cell and adjoining cells.

Figure 1. Schematic of a typical computational volume and cell boundaries.

Equation (1) was integrated over the 'ith' computational cell as follows:

$$\int_{r_{i-1/2}}^{r_{i+1/2}} r dr \rho C_p \frac{\partial T}{\partial t} = \left[r k \frac{dT}{dr} \right]_{r_{i+1/2}} - \left[r k \frac{dT}{dr} \right]_{r_{i-1/2}} + \int_{r_{i-1/2}}^{r_{i+1/2}} r dr q \quad (2)$$

where the volumetric energy generation rate q can follow an exponential form:

$$q = q_o e^{-B(r-r_o)} \quad (3)$$

and where B and r_o are constants determined for the values of q obtained by a two dimensional log-log interpolation at the node boundaries of the supplied spatio-temporal decay heat values. The volumetric energy generation rate q can also follow a piece-wise constant function given by:

$$q = q_i \text{ if } r \in [r_{i-1}, r_i) . \quad (4)$$

Performing the integration assuming q takes the form in Equation (3) and using standard finite difference representations, Equation (2) becomes:

$$\begin{aligned} & \left(\frac{r_{i+1/2}^2 - r_{i-1/2}^2}{2} \right) \rho C_p \frac{(T_i^{n+1} - T_i^n)}{t^{n+1} - t^n} \\ &= r_{i+1/2} k_{i+1/2} \frac{T_{i+1}^{n+1} - T_i^{n+1}}{r_{i+1} - r_i} - r_{i-1/2} k_{i-1/2} \frac{T_i^{n+1} - T_{i-1}^{n+1}}{r_i - r_{i-1}} \\ &+ \frac{q_o e^{-B(r_{i+1/2} - r_o)}}{B^2} (Br_{i+1/2} - 1) - \frac{q_o e^{-B(r_{i-1/2} - r_o)}}{B^2} (Br_{i-1/2} - 1) \end{aligned} \quad (5)$$

where "n" and "n+1" refer to the nth and nth-plus-one solution time advancement.

Equation (5) can be expressed in more compact notation involving the total zone volume:

$$V_i \rho C_p \frac{(T_i^{n+1} - T_i^n)}{t^{n+1} - t^n} = G_{i+1/2} (T_{i+1}^{n+1} - T_i^{n+1}) - G_{i-1/2} (T_i^{n+1} - T_{i-1}^{n+1}) + V_i \bar{q}_i \quad (6)$$

where

$$G_{i \pm 1/2} = \text{thermal conductance between nodes (W/K)}$$

$$V_i = \text{zone volume (m}^3\text{)}.$$

Also, $\bar{q}_i$ is simply a compact representation of the last two terms in Equation (5). If q is given by the piece-wise constant function and is constant during the integration interval, the determination of $\bar{q}_i$ is trivial.

The thermal conductance of Equation 6 is defined as

$$G_{i+1/2} = 2\pi L \left(\frac{r_{i+1/2} k_{i+1/2}}{r_{i+1} - r_i} \right) \text{ and } G_{i-1/2} = 2\pi L \left(\frac{r_{i-1/2} k_{i-1/2}}{r_i - r_{i-1}} \right) \quad (7)$$

where L is the model "effective" height. The volume of 'ith' cell is defined as

$$V_i = \pi L (r_{i+1/2}^2 - r_{i-1/2}^2). \quad (8)$$

1.1 Segment Geometry Specification

The geometry in CHEMCON can be specified for two different radial geometries. This selection only affects the manner in which the total volumes are calculated and has no effect on the underlying numerical scheme.

First, the geometry input can be taken to be the conventional cylindrical shell with a specified height:

$$\text{Area}_1 = 2 \pi R_1 H$$

$$\text{Volume} = \pi (R_2^2 - R_1^2) H$$

The second geometry choice or shell option more closely approximates toroidal shell geometry using circular shell areas with a rotational radius from the toroidal center to the centroid of the circular shell:

$$\text{Area}_1 = 2 \pi R_{\text{rot}} \theta R_1$$

$$\text{Volume} = 2 \pi R_{\text{rot}} (R_2^2 - R_1^2) \frac{\theta}{2}$$

By comparing the inner area and volume formulas between geometry choices, one can define an “effective” height as $H = \theta R_{\text{rot}}$ for the shell geometry choice so that the area and volume formulas for the first or normal cylindrical geometry choice can be used without modification. The user must enter the appropriate value for the effective height such that, depending on what geometry is being modeled, the desired areas and volumes are calculated by the code. Note that the units of θ are radians.

1.2 General Conductance Terms

There are regions of the ITER design where pure conduction is not the applicable mode of heat transfer. For example, the mode of heat transfer between the inboard and outboard side of the reactor is by thermal radiation. To account for the various modes of heat transfer in the problem, models for gap conduction, pebble bed conduction as well as radiation, conduction, convection, and combinations of these modes were included in the CHEMCON code. In this section, the numerical expression for each heat transfer mode is described.

In general, the thermal conductance of Equation 6 takes the following form:

$$G_{i+1/2} = (2\pi L r_{i+1/2} h_{i+1/2}) / M \quad (9)$$

where h_i is a generic heat transfer coefficient ($\text{W}/\text{m}^2 \cdot \text{K}$) and M is the conduction length multiplier. The variation of M allows for modeling highly voided regions as discussed in Reference 2. For a gap conductance boundary condition, the generic heat transfer coefficient is just the value of the gap heat transfer coefficient; i.e., $h_i = h_{\text{gap}}$.

For thermal radiation the radiative heat transfer coefficient is defined as³

$$h_{\text{rad}} = \sigma \epsilon_{\text{eff}} (T_{i+1}^2 + T_i^2) (T_{i+1} + T_i) \quad (10)$$

where

σ = Stefan-Boltzmann constant

ϵ_{eff} = effective emissivity

and where the effective emissivity between the surfaces is

$$\epsilon_{\text{eff}} = \left[\frac{1}{\epsilon_i} + \frac{r_i}{r_{i+1}} \left(\frac{1}{\epsilon_{i+1}} - 1 \right) \right]^{-1} \quad (11)$$

The following correlation is used for natural convective heat transfer within an enclosure:³

$$Nu_{\delta} = 0.42 Ra_{\delta}^{1/4} \left(\frac{\delta}{L} \right)^{1/3} \quad (12)$$

In Equation (12), Nu_{δ} is the Nusselt number based on the characteristic dimension δ (i.e., the gap thickness), Ra_{δ} is the Rayleigh number based on the characteristic dimension δ , and L is the characteristic height.

The following correlation for natural convection from a vertical wall is used for gap boundary conditions that include convection and in the pressurization/condensation single volume model as described in the next subsection:³

$$Nu_L = \left\{ 0.825 + \frac{0.387 Ra_L^{1/6}}{[1 + (0.492/Pr)^{9/16}]^{8/27}} \right\}^2 \quad (13)$$

In Equation (13), Nu_L is the Nusselt number based on the characteristic dimension L (i.e., the characteristic height), Ra_L is the Rayleigh number based on the characteristic height L , and Pr is the Prandtl number of the fluid.

For conduction through a packed pebble bed, the effective thermal conductivity is predicted by the model proposed by Hall and Martin⁴ which is as follows:

$$k_{eff} = \frac{P_f k_g}{0.524} \left[\frac{(\pi/2)(1-\lambda)}{\delta(1-\lambda)-1} - \frac{(\pi/2)(1+m)}{[\delta(1-\lambda)-1]^2} \ln \frac{\delta(1+\lambda m)+m}{(1+\lambda\delta)(1+m)} + (1-\pi/4)(1+\lambda) \right] \quad (14)$$

where

k_b = pebble conductivity (W/m · K)

k_g = gas conductivity (W/m · K)

T = temperature (K)

δ = k_g/k_b

D_p = pebble diameter (m x 10^{-6})

P_g = gas pressure (Pa x 10^6)

m = $3.0833 \times 10^{-4} T^{1.168} / (P_g D_p)$

P_f = packing fraction

λ = $4.4919786 \times 10^{-11} T^{2.332} D_p$.

Thus the heat transfer coefficient for pebble bed conduction would be $k_{eff} / (r_{i+1} - r_i)$.

The following general formula is used to simulate parallel and serial combinations of heat transfer modes:

$$G_{i+1/2} = 2\pi L r_{i+1/2} \sum_j C_j h_j \quad (15)$$

where C_j is the area fraction for the heat transfer modes with a heat transfer coefficients of h_j where modes j take place in parallel.

The pebble bed conduction model includes conduction through structure in parallel with conduction through the pebble bed. Two materials are used for the pebble bed model; the first material is used for the structure material and the second material is used for the pebble material in the pebble bed. The material fraction of each material is used to weight the conductance contribution for conduction and pebble bed conduction respectively.

For parallel conduction and radiation heat transfer modes, the volume fraction of the material is taken as the area fraction for conduction and unity minus the volume fraction is taken as the area fraction for radiation. For parallel convection and radiation in a gap, area fractions are assumed unity for both modes. For the three parallel modes conduction, convection and radiation within a semi-solid region, the conduction area fraction is the volume fraction and unity minus the volume fraction is the area fraction for the modes of convection and radiation.

1.3 Pressurization/Condensation Model

During an in-vessel loss-of-coolant-accident (LOCA), the plasma chamber can be filled with steam and pressurized. The presence of this steam can cause heat transfer to occur which can vary in magnitude with pressure. This heat transfer can take the form of convection and/or mass transfer due to condensation and/or evaporation from hot and cold surfaces in contact with the steam. To include the effects of these heat transfer mechanisms, a single volume model was developed. Figure 2 shows a schematic of the single volume model, the associated upstream and downstream volumes and the solid structures in contact with the single volume.

Figure 2. Schematic of volumes and structures used in the pressurization/condensation model.

This single volume can consist of a two-phase mixture of water and steam with its state consistently determined based on transient energy and mass flows crossing the volume boundaries. The volume boundary is defined by the inboard and outboard first wall and vacuum vessel solid surfaces. In addition, connections to upstream and downstream boundary volumes are allowed. These volumes are designed to represent the blanket coolant volume and the suppression pool volume, respectively.

This single volume model solves the conservation of mass and energy equations. The conservation of mass equation is:

$$V \frac{\partial \rho}{\partial t} = \sum_j (\dot{m}_j^{in} - \dot{m}_j^{out}) \quad (16)$$

The change in mass of the volume includes the mass outflow due to flow to the downstream volume or condensation, and the mass inflow from either the upstream or downstream volumes or evaporation. The conservation of energy for the volume is:

$$V \frac{\partial}{\partial t} (\rho e) = \sum_k \left((\dot{m}_k h_k)^{in} - (\dot{m}_k h_k)^{out} \right) + \sum_n \left(\pm Q_{conv}^n - Q_{cond}^n + Q_{evap}^n \right) \quad (17)$$

The change in energy of the volume includes energy brought in by mass or heat transfer from warmer surfaces minus the energy taken out by mass or heat transfer to colder surfaces. Equations (16) and (17) are also integrated explicitly for the upstream volume to provide a realistic track of the absolute pressure of the upstream volume during blowdown. The upstream volume conditions are not included in the main iteration.

A critical flow model is included in the overall pressurization and condensation model. This model limits flow between all volumes to the critical value based on the upstream volume pressure and quality. The critical flow model is described in Reference 5. This model is based on the Henry-Fauske and HEM

models and can treat conditions from sub-cooled liquid to superheated vapor. Assumptions underlying the model include the following: one-dimensional isentropic flow, slip between phases is negligible, no interphase heat and mass transport between phases during expansion takes place, the liquid phase is incompressible and the vapor phase expands at the throat in a polytropic manner.

The following correlation for the condensation heat transfer coefficient is used:³

$$h_L = 1.13 \left\{ \frac{g \rho_l (\rho_l - \rho_v) k_l^3 h_{fg}}{\mu_l (T_{sat} - T_s) L} \right\}^{1/4} \quad (18)$$

where

- h_L = heat transfer coefficient ($\text{W}/\text{m}^2 \cdot \text{K}$)
- g = gravitational constant = $9.807 \text{ (m/s}^2\text{)}$
- ρ_l = liquid density (kg/m^3)
- ρ_v = vapor density (kg/m^3)
- k_l = liquid thermal conductivity ($\text{W}/\text{m} \cdot \text{K}$)
- h_{fg} = latent heat of vaporization (J/kg)
- μ_l = liquid viscosity ($\text{kg}/\text{m} \cdot \text{s}$)
- T_{sat} = saturation temperature (K)
- T_s = surface temperature (K)
- L = characteristic height (m).

For both the upstream and downstream connections to the single volume, the following equation for mass flow rate is used:⁶

$$\dot{m} = KA|2\rho\Delta P|^{1/2} \quad (19)$$

where

- $\dot{m}$ = mass flow rate (kg/s)
- K = flow coefficient
- A = connection area (m^2)
- ρ = liquid density (kg/m^3)
- ΔP = pressure difference between volumes (Pa).

There are four variables that need to be converged for this model. These are the density and energy of the volume and the inboard and outboard vacuum vessel temperatures. The Newton iteration method used is a simple yet powerful method of solving nonlinear equations. The method consists of simply performing the following numerical calculation for the system function f and its derivative f' using each system parameter u_i until the change in any system parameter is sufficiently small:⁷

$$u_i^{n+1} = u_i^n - \frac{f(u_i^n)}{f'(u_i^n)} \quad (20)$$

The model utilizes the water property set contained in the ATHENA/RELAP5 code.⁸

1.4 Multi-Segment Model

In order to model segments representing different poloidal portions of the first wall/shield blanket, a Multi-Segment model was added to CHEMCON. This model consists of one-dimensional, cylindrical region groups or segments that can be coupled at the innermost or outermost surfaces to the surfaces of other segments. The coupling between segments is numerically explicit with energy deposition occurring within the surface node determined as a function of surface temperatures at the previous time step. In addition, a participating gas consisting of steam can also be modeled.

The following are the set of equations solved for a participating gas in an enclosure:⁹

$$\sum_{j=1}^N \left(\frac{\delta_{kj}}{\epsilon_j} - F_{k-j} \frac{1 - \epsilon_j}{\epsilon_j} \tau_{k-j} \right) q_j = \sum_{j=1}^N (\delta_{kj} - F_{k-j} \tau_{k-j}) \sigma T_j^4 - F_{k-j} \bar{\alpha}_{k-j} \sigma T_g^4. \quad (21)$$

where

δ_{kj} = delta function (unity only when $j=k$, otherwise zero)

ϵ_j = emissivity of surface j

F_{k-j} = view factor between surfaces k and j

τ_{k-j} = transmissivity of path through gas between surfaces k and j

q_j = heat flux on surface j

T_g = temperature of gas

T_j = temperature of surface j

σ = Stefan-Boltzmann constant

$\bar{\alpha}_{k-j}$ = absorptivity of path through gas between surfaces k and j .

The enclosure surfaces and the gas are assumed to be gray. The areas and emissivities for each surface are specified as are the view factors for each radiative path between surfaces. The model for the pressure and temperature dependent steam radiative properties are taken from the TRAC-BD1 computer code.¹⁰

The set of equations represented by Equation (21) are formulated for an enclosure; i.e., the sum of view factors for any given surface is unity. If this sum is not unity, then, effectively, energy is rejected from a surface j to a surface at 0 K with a view factor of unity minus the sum of the view factors for surface j to all other specified surfaces k .

This model has been independently tested for the case without a participating gas. The participating gas option of this model has not been fully tested but will be tested in future versions of the code.

2. OXIDATION REACTIONS

This section describes the correlations used for oxidation reactions between steam and air and the following solid materials: beryllium, graphite and tungsten.

2.1 Beryllium Oxidation

When water contacts a hot beryllium surface, the following oxidation reaction likely occurs:

When air contacts a hot beryllium surface, the following oxidation reaction likely occurs:

The rate at which beryllium-steam reaction proceeds was measured and reported in Reference 11. The beryllium-air reaction rates were obtained from Reference 12. The Arrhenius type oxidation rate relationships ($\text{kg-beryllium}/\text{m}^2 \cdot \text{s}$) developed from these measurements for full density beryllium-air reactions are as follows:

$$R'_{ox} = 2.7 \times 10^{17} e^{-56,300/T} \quad (24)$$

for beryllium-air reactions below 1073 K and

$$R'_{ox} = 11.7 e^{-15,900/T} \quad (25)$$

for beryllium-air reactions above 1073 K. For full density beryllium-steam reactions:

$$R'_{ox} = 1.933 \times 10^6 e^{-25,850/T} \quad (26)$$

for temperatures less than 1173 K, and

$$R'_{ox} = 31.84 e^{-12,830/T} \quad (27)$$

for temperatures greater than 1173 K. A single steam oxidation rate relationship for porous beryllium is available in CHEMCON and is:

$$R'_{ox} = 49.471 e^{-12,500/T} \quad (28)$$

As discussed in References 13 and 14, two derived reaction rate curves are required for best estimate modeling of reaction rates of actual ITER components. For the divertor component, the following log average reaction rate is used:

$$\log R_{ox} = 0.5 \left(\log R_{ox}^{100} + \log R_{ox}^{88} \right). \quad (29)$$

The two reaction rates R_{ox}^{100} and R_{ox}^{88} are the full density and porous reaction rates, respectively.

For the first wall component, the full density reaction rate is used below 773 K and the log average reaction rate is used above 873 K. To bridge these two correlations, the following correlation is used for temperatures between 773 K and 873 K:

$$R'_{ox} = 1.7 \times 10^{15} e^{-41,770/T} \quad (30)$$

The beryllium-steam reaction rates are corrected for pressure dependence as follows:

$$R_{ox} = R'_{ox} P_m \quad (31)$$

where P_m is given by:

$$P_m = \prod_n \left(\frac{\min(P, P_{n+1})}{P_n} \right)^{A_n} \quad (32)$$

P and P_n are the system and reference pressure in MPa and A_n is the multiplier. P_0 and A_0 are 0.086 MPa and 0.9 for pressures less than 0.2 MPa. As the system pressure exceeds 0.2 MPa, 0.4 MPa and 0.6 MPa, the subscript n increases from 1 to 2 to 3, A_n takes on values of 0.6, 0.4 and 0 and P_n takes on values of 0.2 MPa, 0.4 MPa and 0.6 MPa, respectively.

The beryllium-water oxidation reaction is exothermic as is the beryllium-air reaction. The rate at which the chemical energy is generated by this reaction is modeled as a surface heat flux. This heat flux is defined as the difference between the heats of formation of the reactants and products, times the oxidation rate determined from among Equations (24, 25 and 31). Temperature dependent heats of formation were obtained from Reference 15. For beryllium oxide the heat of formation (J/kg-BeO) is:

$$h_{f_{BeO}} = \frac{4187}{M_{BeO}} \left(-144,220 + 0.83T + 0.00046T^2 + 248,000T^{-1} \right) \quad (33)$$

and for water (J/kg-H₂O) is:

$$h_{f_{H_2O}} = -\frac{4187}{M_{H_2O}} \left(56930 + 2.93T + (-0.00064)T^2 + 16000T^{-1} \right) \quad (34)$$

The rate at which energy is released (W/m²) in the beryllium-steam reaction is:

$$q_{ox} = - \left(h_{f_{BeO}} - h_{f_{H_2O}} \frac{M_{H_2O}}{M_{BeO}} \right) \left(\frac{M_{BeO}}{M_{Be}} \right) R_{ox} \quad (35)$$

where M_{BeO} , M_{H_2O} , M_{Be} are the molecular weights of beryllium oxide, water, and beryllium, respectively.

The rate at which energy is released (W/m²) in the beryllium-air reaction is:

$$q_{ox} = -h_{f_{BeO}} \left(\frac{M_{BeO}}{M_{Be}} \right) R_{ox} \quad (36)$$

where M_{BeO} , M_{Be} are the molecular weights of beryllium oxide, and beryllium, respectively.

2.2 Graphite Oxidation

When water contacts a hot graphite surface, the following primary oxidation reaction occurs:

When air contacts a hot graphite surface, the following primary oxidation reaction occurs:

The rate at which the graphite-steam reaction proceeds was measured for various graphites and reported in Reference 16. Reference 17 contains the graphite-air reaction rate measurements. The Arrhenius type oxidation rate relationships ($\text{kg-carbon}/\text{m}^2 \cdot \text{s}$) developed from these measurements for GraphNOL N3M and air are as follows:

$$R_{ox} = 0.12e^{-5,710/T} \quad (39)$$

for temperatures less than 1273 K, and

$$R_{ox} = 0.0076e^{-2,260/T} \quad (40)$$

for temperatures between 1273 K and 2000 K. The Arrhenius type oxidation rate relationships ($\text{kg-carbon}/\text{m}^2 \cdot \text{s}$) developed from these measurements for GraphNOL N3M and steam are as follows:

$$R_{ox} = 8.54 \times 10^7 e^{-35,630/T} \quad (41)$$

for temperatures less than 1460 K, and

$$R_{ox} = 5.18e^{-11,320/T} \quad (42)$$

for temperatures between 1460 K and 2000 K.

The graphite-water oxidation reaction is endothermic while the graphite-air reaction is exothermic. The rate at which the graphite latent energy is consumed or produced by these reactions is modeled as a surface heat flux. This heat flux is defined as the difference between the heats of formation of the reactants and products, times the oxidation rate determined from among Equations (39-42). Temperature dependent heats of formation were obtained from Reference 15. The heat of formation for carbon monoxide (J/kg-CO) is:

$$h_{f_{co}} = -\frac{4187}{M_{co}} \left(25400 + 0.89T + 0.00027T^2 + 219000T^{-1} \right). \quad (43)$$

The rate at which energy is consumed (W/m^2) in the graphite-water reaction is:

$$q_{ox} = - \left(h_{f_{co}} - h_{f_{h_2o}} \frac{M_{H_2O}}{M_{CO}} \right) \left(\frac{M_{CO}}{M_C} \right) R_{ox} \quad (44)$$

where M_{CO} , M_{H_2O} , M_C are the molecular weights of carbon monoxide, water, and carbon, respectively. The rate at which energy is produced (W/m^2) in the graphite-air reaction is:

$$q_{ox} = -(h_{f_{co}}) \left(\frac{M_{CO}}{M_C} \right) R_{ox} \quad (45)$$

where M_{CO} , M_C are the molecular weights of carbon monoxide and carbon, respectively.

2.3 Tungsten Oxidation

When water contacts a hot tungsten surface, the following oxidation reaction occurs:

When air contacts a hot tungsten surface, the following primary oxidation reaction occurs:

The rate at which these reactions proceed was measured and reported in Reference 18. The Arrhenius type oxidation rate relationships ($kg\text{-tungsten}/m^2 \cdot s$) developed from these measurements for tungsten-air reactions is as follows:

$$R_{ox} = 51.35 P_{O_2}^{0.5} e^{-12,170/T} \quad (48)$$

where the pressure of oxygen is in MPa. For tungsten-steam reactions, the reaction rate takes the form:

$$R_{ox} = 136 e^{-15,550/T} \quad (49)$$

The tungsten-water oxidation reaction is slightly exothermic. The rate at which the chemical energy is generated by this reaction is modeled as a surface heat flux. This heat flux is defined as the difference between the heats of formation of the reactants and products, times the oxidation rate determined from among Equations (48 and 49). Temperature dependent heats of formation were obtained from Reference 15. For tungsten oxide the heat of formation ($J/kg\text{-}WO_3$) is:

$$h_{f_{wo_3}} = \frac{4187}{M_{WO_3}} \left(-201,180 + 1.27T + 0.00181T^2 - 60,000T^{-1} \right) \quad (50)$$

The rate at which energy is released (W/m^2) in the tungsten-water reaction is:

$$q_{ox} = - \left(h_{f_{wo_3}} - h_{f_{h_2o}} \frac{3M_{H_2O}}{M_{WO_3}} \right) \left(\frac{M_{WO_3}}{M_W} \right) R_{ox} \quad (51)$$

where M_{WO_3} , M_{H_2O} , M_W are the molecular weights of tungsten oxide, water, and tungsten, respectively.

The rate at which energy is released (W/m^2) in the tungsten-air reaction is:

$$q_{ox} = -h_{f_{wo_3}} \left(\frac{M_{WO_3}}{M_W} \right) R_{ox} \quad (52)$$

where M_{WO_3} , M_W are the molecular weights of tungsten oxide and tungsten, respectively.

3. THERMAL MATERIAL PROPERTIES

Material properties of surface emissivity, density, specific heat, and thermal conductivity for 316 stainless steel, beryllium, beryllium oxide, carbon, copper, inconel, lead, lithium, lithium oxide, tungsten, and vanadium are included in the CHEMCON code. Table 1 contains the equations for these material properties in the CHEMCON code. Note that the porosity is given by the symbol P and the emissivity by the symbol ϵ . Air and water properties are obtained from tables as given in Appendix B.

Table 1. Material Property Table.^{15,19,20}

Material	Density (kg/m^3)	Specific Heat ($\text{J/kg} \cdot \text{K}$)	Thermal Conductivity ($\text{W/m} \cdot \text{K}$)	ϵ
Annealed 316 Stainless Steel	7965.0	$0.4488 + 4.548\text{E-}4 (T-255.4)$ $- 5.966\text{E-}7 (T-255.4)^2$ $+ 3.513\text{E-}10 (T-255.4)^3$, for $300 < T < 1395 \text{ K}$; $285.19 \cdot \log(T) - 233.52$, for $73 < T < 300$	$(1-P) [12.7001 + 1.735\text{E-}2 (T-255.4)$ $- 2.530\text{E-}6 (T-255.4)^2$ $- 1.924\text{E-}10 (T-255.4)^3]$ for $300 < T < 1375 \text{ K}$	0.3
Beryllium	1850.	$2.432 + 6.378\text{E-}4 T - 7.11\text{E-}4 T^2$ for $300 < T < 1556 \text{ K}$	$[(1-P)/(1 + 11 P^2)] 291$ $(1-1.650\text{E-}3 T + 1.464\text{E-}6 T^2$ $- 5.125\text{E-}10 T^3)$ for $300 < T < 823 \text{ K}$	0.6
Lithium Oxide	2033.8	$2.5179 + 3.328\text{E-}4 T - 8.382\text{E-}4 T^2$ for $306 < T < 1073 \text{ K}$	$[(1-P)^{1.96}] [39.79/(1 + 7.067\text{E-}3 T)]$ for $473 < T < 1173 \text{ K}$ and for $0.066 < P < 0.292$	0.6
Beryllium Oxide	2850.0	$1.930 T^{0.326}$, for $400 < T < 2000 \text{ K}$	$(1-P) [42.17 10^{\log(T)}$ $(1.8157 - 0.5997 \log(T))]$ for $300 < T < 1700 \text{ K}$	0.6
Carbon	1800.0	$2000. - 2204. e^{(-0.002028 T)}$ for $300 < T < 3000 \text{ K}$	$(1-P) (35.0 + 251. e^{(-0.001632 T)})$ for $300 < T < 3000 \text{ K}$	0.6
Tungsten	19350.0	$129.8 + 0.0202 (T-300.)$, for $300 < T < 3400 \text{ K}$	$(1-P) (198.1 - 125.5 e^{(-508./T)})$ for $300 < T < 3400 \text{ K}$	0.6
Lithium	505.0	4260.0, for $300 < T < 3400 \text{ K}$	$(1-P) 10^{(27.7134 - 27.8661 T}$ $+ 9.7861 T^2 - 1.1264 T^3)$, for $453 < T < 2200 \text{ K}$	0.1
Vanadium	5960.0	$406.7 + 0.2111 T$, for $475 < T < 2000 \text{ K}$	$(1-P) 10^{(1.680 + 0.1809 T - 0.254 T^2}$ $+ 0.0611 T^3)$, for $453 < T < 2200 \text{ K}$	0.85
Lead	11350.0	$99.7 + 0.08 T$, for $323 < T < 588 \text{ K}$	$(1-P) (39.16 - 0.0133 T)$, for $273 < T < 600 \text{ K}$	0.6
Inconel	8510.0	$350.5 + 0.267 T$, for $273 < T < 1123 \text{ K}$	$(1-P) (5.28 + 0.0145 T)$, for $300 < T < 1600 \text{ K}$	0.2
Copper	8933.0	$39.1 + 2.96 T + (-0.00956) T^2$ $+ (1.493\text{E-}05) T^3$ $+ (-1.1005\text{E-}08) T^4 + (3.085\text{E-}12) T^5$, for $100 < T < 1200 \text{ K}$	320.0, for $166 < T < 1356 \text{ K}$	0.6

4. CODE INPUT/OUTPUT DESCRIPTION

This section describes the philosophy and format of the input file for the CHEMCON code.

4.1 Input Philosophy

The input for CHEMCON is based on the idea of homogeneous regions that can be connected with a variety of boundary conditions. The equation of energy for a node of this homogeneous solid is integrated over the volume of the cell and includes expressions for the energy into and out of the cell at the physical cell boundaries and energy generation due to decay heat or chemical reactions (Equation 6). Each region can possess only one volume fraction value which is the sum of up to two different material fractions.

One heat transfer mode is used for the interior of the region. Different heat transfer modes can be used at the left and right boundaries of the region. A region is connected to adjoining regions through user-defined boundary conditions. For example, regions separated by an evacuated gap would use the radiation heat transfer option to model the heat transfer between these two regions. To model conduction between regions, a large gap conductance (i.e., $> 10^6$ (W/m² K)) and a very small (10^{-6} m) gap can be used to couple the temperatures at the region surfaces and match actual geometry. This small gap and large conductance effectively gives the two region surfaces the same temperature. Note that the heat transfer modes used for adjoining surfaces must be identical.

These regions can be grouped into segments. These segments can communicate at the boundaries with other segments using a radiative boundary condition. The communicating segments must form a complete enclosure; i.e., the sum of the view factors should add to unity.

Generally, the input sequence contains general model information (e.g. transient time, radiation enclosure model specification, etc.) followed by detailed nodal information for each segment (thickness, initial temperature, etc.) as well as transient spatial decay heat information. Distance is input in meters (m), temperature in Kelvin (K), and power in watts (W). Flow coefficients are a function of flow geometry and are used as in Equation (19). For large flow path expansions (i.e., breaks in coolant piping), a value of unity can be used for the flow coefficient as a first approximation.

4.2 Input Description

This section describes the format of the contents of the input file for the CHEMCON code. This file must be named **iter.inp**.

The input is free format but the number and order of fields per line must match that specified in this section. The content and number of the comment lines may be altered as long as the first character is '*'. An example input file is included in Appendix C. Each input line group consisting of comment lines (*italics*) and lines of actual input (**bold**) will be presented in sequence below.

The first input line group simply specifies the total transient time in days for the simulation.

*total transient time in days
100.0

The next input group describes the time step information for the solution of the transient problem.

*number of time control lines

5

*each time control line contains time to start control,

*desired timestep in seconds and output interval in timesteps

0.0 1.0 600

3600. 10.0 360

86400. 120.0 720

1.93e9 180.0 1440

1.96e9 180.0 1440

The next input group specifies whether to print various output files. Note: output files are described in Subsection 4.3.

*flags to toggle printing of (1=yes,0=no):

*3d temps (iter.3dout[n]),

*user temps (user.temps[n]),

*decay heats (iter.udec[n]),

*decay energies (iter.ueng[n]),

*mass temps (iter.tmas[n]),

*total energies (iter.etot[n])

0 1 1 1 1

The next input group specifies the user defined pressure for the model. This pressure is used by the convection heat transfer correlations within a gap and in the beryllium oxidation reaction rates.

*user defined pressure (Pa)

*NOTE this value is overridden if pressure/condensation

*volume model is active (See below)

0.871395e5

The next input group consists of information used for the pressurization/condensation model. This input set was designed to allow the user to model an upstream and downstream volume for the single volume which represents the vacuum vessel interior space. The single volume begins the simulation at a very low pressure with only a tiny amount of water vapor. The parameters for this initial state are limited by the water properties used in the code; i.e., values below the triple point are not allowed.

This input set for this model consists of several lines of input. First, a model status flag is entered. It must be noted that the single volume model is incompatible with the use of heat transfer option 7 anywhere within the model because of the necessity of using a consistent property set for the single volume.

**next set of input is for the condensation/pressurization model

*when enabled, this model overwrites user-defined pressure

*this model is incompatible with gap convection heat transfer flag (7)

*

*pressurization/condensation model initial status (1=on,0=off)

*time to switch status

0 1.e9

The next line of input is the convergence criteria. This quantity determines the maximum error allowed in the quantities used in the single model; i.e, volume density, volume energy, and the inboard and outboard surface temperatures.

* convergence criteria (suggested value 1.e-6)

1.e-5

The next line of input concerns the upstream volume. This volume is meant to allow the user to simulate the blanket coolant system. The user is required to input the upstream pressure, the area connecting the upstream volume to the single volume, the friction coefficient for this connection, the temperature of the upstream volume, the delay for opening this connection and the total upstream liquid mass. The delay entered here is meant to simulate the possible delay in first wall melting that could occur in a LOCA simulation. The total upstream liquid mass serves to limit the total amount of liquid that spills into the single volume. The flow between these volumes is calculated as described in Section 1.3.

*upstream volume conditions (blanket loop)

*pressure (Pa), connection area (m²), flow coefficient, temperature (K)

*delay for blanket spill (s) blanket coolant mass (kg)

2.8e6 5.e-4 1.0 473. 120. 1.153d5

The next line of input for the single volume model is used for the downstream volume. This volume is designed to allow the user to simulate the suppression tank. The input required consists of the pressure for the downstream volume, the connection area between the single volume and the downstream volume, the friction coefficient for this connection, the enthalpy of the fluid mixture in the downstream volume, the pressure for rupture disk failure, and the initial connect status of the two volumes. The enthalpy of the downstream volume is needed to model the energy content of any flow from the downstream volume back into the single volume. The pressure for rupture disk failure value is used to simulate the behavior of a rupture disk by keeping the connection closed until this absolute pressure is exceeded. When this condition occurs, the connection remains open indefinitely. Normally, the connection status would be closed until opened by the single volume pressure exceeding the rupture disk failure pressure, but the user can simulate an initially open connection as well.

*downstream volume conditions (suppression pool)

*pressure (Pa), connection area (m²), flow coefficient, enthalpy (j/kg)

*pressure for rupture disk failure and initial connect status (1=open,0=closed)

0.1e6 0.1 1.0 2.676e6 1.7e5 0

The final input set consists of information specifying the system parameters to be included in the convergence algorithm. This includes surfaces in contact with the pressurization/condensation volume, and which surface temperatures are to be used in the Newton iteration scheme. Normally, only temperatures of surfaces upon which condensation is expected are included since the system state depends strongly on these

temperatures. The surfaces upon which condensation is not expected can be omitted from the iteration since they likely will not change drastically with changes in the state of the pressurization/condensation volume.

**next set of input describes connecting surfaces
*to the single volume in the pressurization/condensation model
*first line is number of surfaces in contact with volume
*next line(s) consist of
*1)segment id
*2)region id
*3)inner=1, outer=2 side of surface
*4)allow convection at surface (0=no,1=yes)
*5)allow condensation at surface (0=no,1=yes)
*6)converge on surface temperature (0=no,1=yes)
*note: normally only condensation surfaces need
*to be converged upon; i.e., flag5 >= flag6

4
1 26 2 1 0 0
2 1 1 1 0 0
1 8 2 1 1 1
2 19 1 1 1 1

The next input group specifies the radiation enclosure model surfaces and geometry.

*next set of input is for the radiation enclosure model
*this model can include a participating gas
*the participating gas option is currently not available
*
*number of segments participating in enclosure model (<= 8)
*flag to turn enclosure model on(=1) or off(=0)
*and gas participation (0=no, 1=yes)

3 1 0
*segment numbers for each participating segment
1 2 3
*inner(=-1) or outer(=1) surface for each segment
1 -1 -1

*emissivity of each surface
0.6 0.6 0.6

*area of each surface
350. 350. 350.

*next n lines are the view factor matrix:
*view factor from 1 to 1, 1 to 2, etc. across
*view factor from 1 to 1, 2 to 1, etc. down

0.0 0.8 0.2
0.8 0.0 0.2
0.2 0.2 0.6

*next n lines are the path length matrix:
*path length from 1 to 1, 1 to 2, etc. across
*path length from 1 to 1, 2 to 1, etc. down
5.0 5.0 5.0

5.0 5.0 5.0
5.0 5.0 5.0

The next input group specifies the properties for a user defined material.

*first line contains number of user defined materials ($1 \leq n \leq 10$)
*next n lines contains user defined material properties
*specific heat, density, thermal conductivity and emissivity
*note: user defined material indices range from 20 to 29
2
644.5 7965. 27.24 0.2
100. 1000. 100. 0.1

The next input group specifies the emissivity for each material. For reference, the comment lines following the emissivity input gives an index for the heat transfer modes available.

The heat transfer modes are combined as described in Section 1.2. The heat transfer modes available are as follows: 1) pure conduction, 2) conduction and radiation within a region with a material fraction less than unity, 3) conduction, radiation and convection within a region with a material fraction less than unity, 4) gap conduction with a specified gap conductance applied at a region surface only, 5) radiation applied at the region surface only, 6) pebble bed conduction, 7) convection and radiation applied at a region surface only, 8) foil model applied at region surface only with specified foil model input (see below), 9) conduction and radiation within a region with a material fraction less than unity and line-of-sight radiation between region surfaces, 10) user defined gap conduction and standard radiation applied at a region surface only.

*next three lines contain material index and emissivity
*1 2 3 4 5 6 7 8 9 10 11 12 13
*ss be lio2 beo c w air stm li v pb incl cu
0.20 0.60 0.60 0.60 0.60 0.60 0.0 0.0 0.10 0.85 0.60 0.20 0.60
*next eight lines contains heat transfer mode index reference
*1-cond 2-cond+rad 3-cond+rad+conv 4-gap
*5-rad 6-pebble bed 7-conv+rad 8-foil model
*note: flag 8 requires additional input as described after region input
*9-cond+rad (rad heat transfer is line-of-sight
*between inner surface and outer surface of region
*10-gap cond+rad (user defined gap conductance parallel with rad)
*note: flags 4, 5, 7, 8 and 10 should be used only for boundary conditions

The next input group specifies the number of segments in this model.

*number of segments in model (≤ 8)
3

The next input group specifies a multiplier to be applied to the transient decay heat values. This has been included to allow for parametric heat studies without changing decay heat input.

*BEGIN SEGMENT INPUT

*decay heat multiplier set 1

*time to switch multiplier from set 1 to set 2

*(set time equal to zero for set 1 only)

*decay heat multiplier set 2

1.0 0. 1.0

The next two input groups specify the boundary condition to be used for the inner and outer surface of this segment.

*left (inner) boundary condition flag

*0=insulated, -1=fixed temp, or -2=heat flux

*boundary temperature or heat flux (always required)

0 293.

*right (outer) boundary condition flag

*0=insulated, -1=fixed temp, or -2=heat flux

*boundary temperature or heat flux (always required)

0 293.

The next input group specifies the starting radius for this segment.

*starting radius

1.e-6

The next input group specifies the effective height for this segment.

*effective height

11.72

The next input group gives the total number of regions used in this segment.

*total number of regions

54

The next input group consists of detailed region input. Note that region string identifiers are required for each region; i.e., they are not considered comments.

*** region input ***

*each region input consist of three or more lines

*first line contains region character string id

*the next line contains the following fields:

*1) gap thickness preceeding region,

*2) gap conductance

*3) region thickness

*4) number of nodes in region

*5) boundary heat transfer mode for inner node

*6) heat transfer mode for middle nodes

*7) boundary heat transfer mode for outer node
 *8) initial surface temperatures for region
 *9) conduction length multiplier for region
 *10) number of region materials
 *the next one or two lines contain the following fields:

*1) material id for each material
 *2) volume for each material
 *3) power fractions for each material
ib buckling cylinder - region 1
 1.e-6 1.e6 2.06 2 1 1 4 4.5 1.0 1
 1 1. 1.

ib solenoid - region 2
 1.e-6 1.e6 0.815 2 4 1 4 4.5 1.0 1
 1 1. 1.

ib tf magnet - region 3
 1.e-6 1.e6 0.895 2 4 1 8 4.5 1.0 1
 1 1. 1.

ib tf foils outer - region 4
 0.065 3.e3 0.0005 2 8 1 8 77. 1.0 1
 1 1. 1.

ib gamma shield - region 5
 0.065 3.e3 0.030 2 8 1 4 77. 1.0 1
 1 1 1. 1.

The next input group consists of user specified temperatures to be output.

*next four lines contain info to define user defined temperature output
 *first line contains the integer number of different regions (≤ 8)
 *second line contains list of integers identifying each region
 *third line contains the number of temperatures points per region (total ≤ 8)
 *fourth line contains integer identifiers for each node within a region

3
 8 9 26
 1 1 1
 2 1 2

The next input group specifies the regions for the boiling model. This model is intended to model the energy removed from the first wall and/or blanket as a stagnant coolant system boils off. Relief valve information is required to model its periodic opening and closing behavior. It must be noted that the boiling model is incompatible with the use of heat transfer option 7 anywhere within the model because of the necessity of using a consistent property set for the single volume. A value of unity can be used for the valve flow coefficient as a first approximation in the absence of valve design information from the valve manufacturer.

*number of region sets to be boiled (≤ 8)
 1
 *beginning and ending regions for each boiling region set
 *and on/off flag (0=off, 1=on)

9 20 1

**temperature, pressure, relief valve area,
*valve flow coefficient, heat transfer coefficient,
*internal blanket area, blanket liquid mass and
relative lower and upper pressure setpoint
410. 3.e6 1.e-2 1.0 100. 100. 2.5e5 1.05 1.1

The next input group consists of input for the auxiliary cooling/heating model. This model assumes that the nominal amount of power entered for each group is the total amount in watts. This power is spread evenly over the user-specified region group associated with the input power. The nominal rejection and region temperatures are used to determine cooling according to $[(T - T_{\text{rejection}})/(T_{\text{region}} - T_{\text{rejection}})]Q_{\text{nominal}}$. Note that if Q_{nominal} is less than zero, the region group specified will be cooled. If Q_{nominal} is greater than zero, the region group specified will be heated. The energy added to a region group can also be held constant. Finally, a single trip time is allowed for each region group.

*number of auxiliary regions to be cooled/heated (≤ 8)
1
*auxiliary cooling flags (1=on, 0=off)
1
**time to toggle flags
1.e9
*use constant (=0) or variable (=1) type energy term
1
beginning and ending regions to be cooled/heated for each region group
6 8
*nominal power for each region group (W)
-0.75e6
*nominal rejection temps
373.
*nominal region temps
423.

The next input group consists of foil model information. The foil model uses the number of foils, foil emissivity and gap conductance entered to calculate the heat transfer coefficient from one region to another when the gap between these regions contains a thermal shield. When the collapsed area equals zero, a radiation heat transfer coefficient is calculated and divided by the number of foils in the gap plus one. When the collapsed area is non-zero, the radiation heat transfer coefficient and the gap conductance heat transfer coefficient are weighted by the uncollapsed and collapsed areas respectively. Then, by dividing by the number of collapsed foils, the effective heat transfer coefficient for the collapsed foils is determined. The radiation heat transfer coefficient for the uncollapsed foils is then determined using the number of uncollapsed foils as described above. The foils are collapsed one at a time starting at 95% of the collapse temperature with all foils collapsing at the collapse temperature. By using a collapse temperature that is higher than expected temperatures during the transient, the foils can be prevented from collapsing in any of the specified regions.

*segment, region and node number for temperature

*to control foil collapse

1 8 2

*number of regions with foils in preceding gap (<=8)

1

*region numbers

4

*number of foils preceding region

15

*emissivity of each foil group

0.08

*temperature for collapse of foils

3773.0

*fraction of foil area that collapses

0.7

The next input group consists of oxidation model information.

*gas name (air=0 or stm=1)

1

*oxidation flag (1=on,0=off) and to which region surfaces to apply oxidation model

*(-1=inner surface, 1=outer surface, 0=both surfaces)

1 1

*next line contains rate flag and multiplier

*rate flag (0=full density, 1=12% porous,

*rate flag 2=geometric mean of full and porous (Divertor),

*rate flag 3=full density below 773 K,

*rate flag geometric mean above 873 K,

*rate flag interpolated between 773 K and 873 K (First Wall)

*rate flag 4=user input multiplicative (M) and exponential (E)

*rate flag constants; i.e., $M \times \exp(-E/T)$ where T = temperature

*rate flag (NOTE: flag 4 requires extra line for two constants)

*multiplier: multiply reaction rate regardless of porous flag option

0 1.0

*region to apply oxidation model

26

The next input group consists of region numbers to indicate over which regions the user wishes to integrate decay heat for output.

*next set of input specifies regions for decay heat integration

*number of region groups to input (<=8)

1

*beginning and ending region numbers

1 26

The next input group contains transient decay heat data. The zero radius for the spatial decay heat point is determined by the user.

*decay heat transient data

*first line has three inputs:

*1) is the decay energy distribution type

*decay (0) assumes spatial decay between points and integrates

*discrete (1) changes at entered points in stairstep fashion

*2) is which region index to start as $r=0$

*3) is which direction to increment decay spatial coordinate

* 0=inner to outer, 1=outer to inner

*rest of decay data is arranged as follows:

*1) number of time points, number of space points

*2) radii entered starting from first wall armor ($r=0.0$)

*3) time value

*4) decay heat values entered corresponding to each space point

*(repeat 3 and 4 for each time point)

1 26 1

8 12

0.0 0.0020005 0.0090015 0.0100025 0.0630035 0.0730045 0.0780045

0.180 0.282 0.384 0.486 0.4861

.000000E+00

.93200000E+05 .81000000E+06 .18700000E+06 .14800000E+06 .88000000E+05

.73000000E+05 .31592732E+05 .70896111E+04 .15658062E+04 .34666319E+03

.000001E-09 .000001E-09

The input for each segment is repeated starting from the decay heat multiplier input group to the decay heat transient input group.

4.3 Output Description

There are a variety of output files produced by CHEMCON. First, the input is echoed in the file **echo.inp**. A detailed geometric output is produced in **geo.nodes**. This file contains the cell radial boundaries for each cell. It also shows the region accounting done in the code and is useful when trying to determine the region number assigned to each region by CHEMCON. The output file **iter.gas** contains the time in days in column 1, the amount (kg) of hydrogen and carbon dioxide produced during the transient in columns 2 and 3, the thickness (m) of material oxidized in column 4. These quantities are summed over all segments. The output file **iter.radnet** contains the net total energy (W) applied to each segment surface participating in the enclosure model.

The **iter.out** output file contains a variety of information. First, the thermal properties for the 13 standard materials are printed out from 300 K to 1700 K. Next, a segment-by-segment, cell-by-cell printout of the material number, inner radius, thickness, volume, initial temperature, initial decay heat density, initial total decay heat and running sum of total decay heat. Next, a small printout of the total masses for each decay heat region in each segment. Finally, for each time step output interval specified at the beginning of the input file and for each cell in each segment, a printout of the cell inner radius, the product of the heat transfer coefficient and area for the inner and outer cell surfaces, the product of the three quantities: cell

density, cell specific heat and cell volume, the energy generation density, and the relative difference in energy leaving the outer surface of the previous cell and entering the inner surface of the current cell. The last column is used primarily for ensuring the same heat transfer mode is used for adjoining cell surfaces and should normally be zero for complete energy conservation between cells.

The next set of output files concerns the pressurization/condensation model. The first column for all these files contains time. The file **iter.econ** contains the integrated net energy gain (W) by the single volume. The file **iter.mcon** contains the integrated condensed liquid mass (kg) and the total water mass (kg) in the vacuum vessel. The file **iter.pcon** contains the pressure (Pa) of the single volume and of the upstream volume. The file **iter.qcon** contains the steam quality of the single volume. Finally, the file **iter.tcon** contains the temperature (°C) for the single volume and upstream volume.

For this final set of output files, there is an additional output file produced with each defined segment. There are two temperature output files produced: **user.temps** and **iter.3dout**. The file **user.temps** contains the user defined temperatures (°C) in columns with the first column being time (days). The file **iter.3dout** contains the temperatures at each node location through time. The columns are radius (m), time (days) and temperature (K). The output file **iter.udec** contains the user defined decay heat (W) output for each user defined region group with the first column being time (days). The output file **iter.ueng** contains the user defined integrated decay heat output in each column with the first column being time (days). The final column in this file is the total integrated decay heat for all regions (MJ). The output file **iter.etot** contains the total energy change (J) from time zero for each decay heat region specified. The output file **iter.tmas** contains the mass-averaged temperature (K) for each decay heat region specified. The mass-averaged temperature is the product of the temperature and mass of each cell summed over all cells and divided by the total mass.

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APPENDIX A

CHEMCON Code Testing

A-1 CODE MODIFICATION HISTORY SINCE CHEMCON 2.0

CHEMCON 2.1 - A feature to set inner and outer boundary conditions to a user specified heat flux or temperature has been added. This is implemented using a boundary condition flag of -1 or -2, respectively.

CHEMCON 2.2 - The pressurization model has been enhanced by adding a numerically explicit procedure for tracking of mass density and total energy for the upstream (coolant) volume. This feature should provide a more realistic pressure differential estimate between this volume and the plasma chamber volume during blowdown. In addition, a choking model has been added that limits break flow between any two volumes to the critical value.

CHEMCON 2.8 - The air reaction rates developed previously were added for the first wall materials of beryllium, graphite and tungsten.

CHEMCON 2.9 - A feature to allow a volume of coolant in contact with user specified regions to somewhat realistically boil away was added. Flow parameters for the release path are included in the model.

CHEMCON 3.0 - The multisegment feature was added in this version of the code. This feature allowed the user to define multiple segments as parts of an enclosure. These segments communicated through thermal radiation boundary conditions at their inner and/or outer boundaries.

A-2 TESTING OF NEW FEATURES IN CHEMCON 2.2

This section describes the verification actions taken to verify the new features in the CHEMCON Version 2.2 computer code.

A-2.1 Testing of the conduction length multiplier feature

Reference A-1 describes the results of a comparison of spatial temperature distributions for a simplified model of the ITER blanket. The temperatures obtained using the one-dimensional model used in CHEMCON were compared against those obtained using a two-dimensional finite element model. It was found that the one-dimensional results could be brought into agreement with the two-dimensional results within a few percent using a conduction length multiplier. This task verifies the conduction multiplier feature added to the CHEMCON code.

Duplicating the model in Reference A-1, the steady spatial distribution of temperatures obtained from CHEMCON 2.2 was compared against those obtained from the modified version of CHEMCON used in Reference A-1. The results were different by less than two percent. There are two reasons for the differences. First, the previous work used a constant average thermal conductivity in the formulation of the heat flux boundary condition. In addition, the boundary condition was applied using the first two boundary nodes rather than applying the heat flux at the surface. The uncorrected steady state temperature was 612 K rather than the 600 K reported in Reference A-1. Applying the conduction multipliers of 2.3 and 3.1 successively gave peak temperatures within 2 percent of the temperatures obtained from the two-dimensional model as reported in Reference A-1.

A-2.2 Testing of the new beryllium-steam reaction rate equations

To verify these equations, a CHEMCON input deck was constructed that consisted of two beryllium regions; one representing the inboard first wall armor and one representing the outboard first wall armor region. The boundary conditions applied to the inner and outer surface of the model were constant temperature of 700, 800, and 900 K. Various pressures chosen from among 0.05, 1.0, 3.0, 5.0, and 7.0 MPa were used at each temperature.

Ten cases were run, each for 0.01 days, using the first wall option for the beryllium steam reaction rate. This option utilizes the full density, interpolated, and log average reaction rate correlations. Comparisons of the rates derived from the total hydrogen produced for each case with hand calculations were within 1%.

The individual options of full density and divertor (log average) were tested and gave results at pressures of 0.1 MPa and 0.3 MPa that were within a few percent of independent hand calculations. Finally, the porous option was run and the results compared well with hand calculations. These results were also successfully duplicated using the user specified constants for a temperature dependent oxidation option. It must be noted that coding errors were uncovered during the testing of these features and the use of the new oxidation options in CHEMCON 2.0 is not recommended. The coding has been corrected as of CHEMCON version 2.2.

A-2.3 Benchmark of the pressurization/condensation model against the MELCOR code

The purpose of this task is to compare the pressurization trends predicted by CHEMCON 2.2 with trends obtained with the more sophisticated computer code MELCOR. To test this rapid transient, a blowdown of a 125 m³ of 2.0 MPa water will be simulated.

For this task, a MELCOR test problem consisting of three volumes and two fixed temperature surfaces was constructed. One volume represents a coolant volume and is called the upstream volume in CHEMCON. This volume is initially at 2 MPa pressure and 473 K temperature. The second volume represents the plasma chamber. This volume is initially at 1 kPa and is in contact with the first wall surface at a constant 633 K and the vacuum vessel surface at a constant 423 K. The third volume represents the suppression tank and is at saturated conditions for a pressure of 0.1 MPa. In MELCOR the suppression tank volume is modeled as a time independent volume to match the CHEMCON treatment of this model. This last volume is called the downstream volume in CHEMCON.

To prepare the test case for CHEMCON, a few code modifications were performed. First, in CHEMCON 2.0, the coolant volume was at a fixed pressure. This modeling assumption likely results in an overestimate of the break flow. To make this volume model more realistic, a simple numerically explicit tracking of the upstream volume density and energy was implemented along with a choking model that limits the break flow to the critical value for the upstream volume conditions. This choking model is also applied at the connection between the plasma chamber volume and the suppression tank volume and uses the plasma chamber conditions to determine the choking limit for flow between these two volumes.

The critical flow model is described in Reference A-2. This model is based on the Henry-Fauske and HEM models and can treat conditions from sub-cooled liquid to superheated vapor. Assumptions underlying the model include the following: one-dimensional isentropic flow, slip between phases is negligible, no interphase heat and mass transport between phases during expansion takes place, the liquid phase is incompressible and the vapor phase expands at the throat in a polytropic manner.

For the test problem, a 0.468 m thick stainless steel region is used in place of the normal first wall and blanket regions. This is done to ensure a steady temperature of 633 K for the first 1000 s of the transient. The vacuum vessel regions are modeled with very thin 1 micron thick steel regions. This allows the inner and outer boundary conditions at constant temperature of 423 K to be seen by the plasma chamber volume. All regions are thermally insulated from each other through the use of a very low coupling gap conductance value.

The transient is a break of the first wall at 100 s and the rupture disk is set to break at a 0.2 MPa pressure gradient in MELCOR and at 0.3 MPa absolute pressure in CHEMCON. Figure A-1 shows the pressure curves for the coolant and plasma chamber volumes for both the MELCOR model and the CHEMCON model. The transient pressure trends of MELCOR are matched fairly well by the CHEMCON code. The peak pressure in the plasma chamber predicted by MELCOR is 0.505 MPa while that predicted by CHEMCON is 0.393 or 22% lower. This difference is within the engineering uncertainty of the models.

A-2.4 Testing of the vertical wall convection correlation

This correlation is described in the CHEMCON user's manual. To verify the vertical wall convection correlation, the constant pressure convection/radiation heat transfer flag (option 7) was chosen for a gap between regions. Then a pressure of 0.1 MPa was input as the user defined pressure. An inner boundary condition of 1000 W/m^2 and an outer boundary condition of 373 K were used on a five region CHEMCON model identical to that used in Reference A-1. The gap convection and radiation heat transfer flag was used between the third solid region and the highly voided region preceding it. To restrict the heat transfer within the gap to the convection, the emissivity of the stainless steel material was set to $1.e-9$.

The heat transfer coefficient reported for this gap was $4.9 \text{ (W / K m}^2\text{)}$ using an average temperature of 470 K. This coefficient was checked against hand calculations employing the original correlation from reference A-3 and was within a few percent. Finally, the coding was inspected and this same vertical wall convection correlation is used in the pressurization and condensation model for convection heat transfer.

A-2.5 Testing of the air oxidation reaction rate equations

To verify these equations, a CHEMCON input deck was constructed that consisted of a single beryllium region representing the first wall armor. The boundary conditions applied to the inner and outer surface of the model were constant temperature of 700, 800, 900, and 1300 K. Two pressures of 1 atm and 0.25 atm at 1300 K were for tungsten since it was the only material with a pressure dependent air reaction rate. Each case was run for 0.01 days. Comparisons with hand calculations of the total thickness of first wall material reacted for each case were within 1%.

A-2.6 Testing of the boiling model

The boiling model was tested by comparing the total energy change within a 200,000 kg blanket volume to the total energy applied to the blanket volume. A very thin 1 mm stainless steel solid with 1200 m^2 of surface area was subject to 5000 W/m^2 applied to over 0.196 days. The total integrated energy equaled the energy change of the blanket volume over this time within 1%. The energy storage within this thin stainless steel solid was negligible.

A-2.7 Testing of the multisegment model

This section describes the testing of the multi-segment radiation coupling model testing. A 2-D finite element model was developed using the FIDAP computer code. This model was based on a cross section of a vertical cut through the torus and followed the contours of the plasma facing surface (first wall) and the divertor. An arbitrary 10 cm thick stainless steel material was used to give the surface some thickness. This finite element model was used to determine the element-length-averaged view factors for the four plasma facing surfaces approximated in the CHEMCON test problem. Four sections were defined as representing the vertical portion of the inboard, the vertical portion of the outboard, a horizontal section of the top of the first wall and the divertor.

Since, the view factor calculation is not exact, the view factors do not add to unity. At first it was thought that the residual view factor (i.e. $1 - \text{sum of the viewfactors for surface } n$) could be added to the self view factor for each surface to enforce closure and reciprocity simultaneously. However, this change actually made the energy balance among the surfaces (ideally identically zero) worse; i.e., the balance was 0.5% with the non-unity view factors and almost 6% with the "corrected" view factors. Taylor⁴ found similar behavior with inexact view factor calculations and recommends a procedure to alleviate this effect. Hence, it is recommended that this reference be used when new models demand the calculation of new view factors. For example, use of the Leersum procedure to adjust the view factors results in improvement of the energy balance for this test problem to within 0.01%. However, the inexact view factors will be used given the acceptable energy balance achieved using them.

For the CHEMCON test problem, the three first wall back surfaces were fixed at 1273 K while the divertor back surface was fixed at 373 K. Total energy values for the four segments were checked independently using a spreadsheet and were within 1% of the independent values. At this time, the participating medium option has not been tested and should not be used for safety analyses.

A-3 TESTING OF CHEMCON 2.2 ON THREE COMPUTER HARDWARE PLATFORMS

The benchmark problem employing the multi-segment model was run on three different computer platforms. The code was developed on a HP735 computer running HP/UX 9.03. The code was ported to an IBM PowerStation 370 with the latest FORTRAN compiler xlf90. The code was compiled and linked with the new FORTRAN libraries to produce a transportable executable. The benchmark problem was run on the IBM 370 and produced identical results to those seen on the HP735 computer. The executable was then moved to an IBM 590 without the new compiler. The executable was run and produced identical results.

A-4 REFERENCES

A-1. M. J. Gaeta and G. L. Hawkes, "Investigation of the Two-Dimensional Effect on the One-Dimensional Conduction Model for the ITER Outline Design," ITER/US/95/TE/SA-01, January 27, 1995.

A-2. C. G. Bruch, "RELAP4/MOD5: A Computer Program for Transient Thermal-Hydraulic Analysis of Nuclear Reactors and Related Systems; User's Manual Volume 1: RELAP4/MOD5 Description", SRD-113-76, Aerojet Nuclear Company, June 1976.

A-3. F. P. Incropera and D. P. DeWitt, "Fundamentals of Heat Transfer," John Wiley and Sons, New York, 1981.

A-4. R. P. Taylor and R. Luck, "Comparison of Reciprocity and Closure Enforcement Methods for Radiation View Factors", ASME/JSME Thermal Engineering Conference 1995, ASME, 1995.

Figure A-1. Pressure transient comparison for coolant volume blowdown into plasma chamber.

APPENDIX B

Air and Steam Temperature Dependent Property Tables

Volumetric Expansion Coefficient Tables (1/K)

c Data Pairs (T(K), 1/K)

data bgair / 273.2,1.13e-3, 310.9,9.94e-4, 366.5,8.44e-4,
1 422.0,7.33e-4, 477.6,6.44e-4, 533.2,5.78e-4, 588.7,5.24e-4,
1 699.8,4.41e-4, 810.9,3.81e-4, 1088.,2.83e-4 /

c

c Data Pairs (T(K), 1/K)

data bgstm / 373.2,8.28e-4, 422.0,7.33e-4, 477.6,6.44e-4,
1 533.2,5.78e-4, 588.7,5.24e-4, 699.8,4.41e-4, 810.9,3.81e-4,
1 1088.,2.83e-4 /

Specific Heat Tables (J/kg · K)

c Data Pairs (T(K), J/kg/K)

data cpair / 273.2,1004.9, 310.9,1004.9, 366.5,1009.0,
1 422.0,1017.4, 477.6,1025.8, 533.2,1034.2, 588.7,1046.7,
1 644.3,1059.3, 699.8,1071.8, 755.4,1084.4, 810.9,1096.9,
1 1088.,1155.6 /

c

c Data Pairs (T(K), J/kg/K)

data cpstm / 373.2,1888.3, 422.0,1909.2, 477.6,1934.3,
1 533.2,1967.8, 588.7,1997.2, 644.3,2030.6, 699.8,2068.3,
1 755.4,2093.5, 810.9,2135.3, 922.0,2219.1, 1033.,2302.8,
1 1144.,2344.7, 1255.,2428.4 /

Viscosity Tables (N · s/m²)

c Data Pairs (T(K), kg/m-s)

data mugair / 272.2,1.71e-5, 310.9,1.90e-5, 366.5,2.16e-5,
1 422.0,2.38e-5, 477.6,2.59e-5, 533.2,2.78e-5, 588.7,2.98e-5,
1 699.8,3.33e-5, 810.9,3.66e-5, 1088.,4.35e-5 /

c

c Data Pairs (T(K), kg/m-s)

data mugstm / 373.2,1.30e-5, 422.0,1.43e-5, 477.6,1.62e-5,
1 533.2,1.83e-5, 588.7,2.04e-5, 699.8,2.43e-5, 810.9,2.83e-5,
1 1088.,3.83e-5 /

Density Tables (kg/m^3)

c Data Pairs (T(K), kg/m3)

data rhoair / 273.2,1.297, 310.9,1.137, 366.5,0.977,
1 422.0,0.833, 477.6,0.737, 533.2,0.659, 588.7,0.597,
1 644.3,0.546, 699.8,0.503, 755.4,0.466, 810.9,0.434,
1 1088.,0.324 /

c

c Data Pairs (T(K), kg/m3)

data rhostm / 373.2,0.595, 422.0,0.525, 477.6,0.461,
1 533.2,0.413, 588.7,0.373, 644.3,0.341, 699.8,0.314,
1 755.4,0.290, 810.9,0.271, 922.0,0.239, 1033.,0.213,
1 1144.,0.192, 1255.,0.175 /

Thermal Conductivity Tables ($\text{W/m} \cdot \text{K}$)

c Data Pairs (T(K), W/m/K)

data tcair / 273.2,0.0242, 310.9,0.0267, 366.5,0.0301,
1 422.0,0.0334, 477.6,0.0367, 533.2,0.0399, 588.7,0.0433,
1 644.3,0.0464, 699.8,0.0495, 755.4,0.0524, 810.9,0.0552,
1 1088.,0.0692 /

c

c Data Pairs (T(K), W/m/K)

data tcstm / 373.2,0.0251, 422.0,0.0296, 477.6,0.0346,
1 533.2,0.0395, 588.7,0.0445, 644.3,0.0498, 699.8,0.0556,
1 755.4,0.0614, 810.9,0.0672, 922.0,0.0791, 1033.,0.0917,
1 1144.,0.1056, 1255.,0.1177 /

APPENDIX C

COMPLETE INPUT MODEL REFERENCE

```

*VERSION 3.1 INPUT
*total transient time in days
1.000
*number of time control lines
6
*each time control line contains time to start control,
*desired timestep in seconds and output interval in timesteps
0.0      1.0    30
360.     2.0   180
3600.    3.0   180
86400.   9.0   720
864000.  27.0  720
1.96e9  100.0 1440
*flags to toggle printing of:
*3d temps      (iter.3dout[n]),
*user temps    (user.temps[n]),
*decay heats   (iter.udec[n]),
*decay energies (iter.ueng[n]),
*mass temps    (iter.tmas[n]),
*total energies (iter.etot[n])
1 1 1 1 1 1
*user defined pressure (Pa)
*NOTE this value is overridden if pressure/condensation
*volume model is active (See below)
0.871395e5
*next set of input is for the condensation/pressurization model
*when enabled, this model overwrites user-defined pressure
*this model is incompatible with gap convection heat transfer flag (7)
*
*pressurization/condensation model initial status (1=on,0=off)
*time to switch status
0 1.e9
* convergence criteria (suggested value 1.e-6)
1.e-5
*upstream volume conditions (blanket loop)
*pressure (Pa), connection area ( $\pi^2$ ), flow coefficient, temperature (K)
*time for blanket spill (s) blanket coolant mass (kg)
2.e6 1.0 1.0 473. 10. 1.25d5
*downstream volume conditions (suppression pool)
*pressure (Pa), connection area ( $\pi^2$ ), flow coefficient, enthalpy (j/kg)
*pressure for rupture disk failure and initial connect status (1=open,0=closed)
0.1e6 10. 1.0 2.676e6 0.17e6 0
*next set of input describes connecting surfaces
*first line is number of surfaces in contact with volume
*next line(s) consist of
*1)segment id
*2)region id
*3)inner=1, outer=2 side of surface
*4)allow convection at surface (0=no,1=yes)
*5)allow condensation at surface (0=no,1=yes)
*6)converge on surface temperature (0=no,1=yes)
*note: normally only condensation surfaces need
*to be converged upon; i.e., flag5 >= flag6
4
1 26 2 1 0 0
2 1 1 1 0 0
1 8 2 1 1 1
2 19 1 1 1 1

```

```

*next set of input is for the radiation enclosure model
*this model can include a participating gas
*to use participating gas the pressurization/condensation
*model must be active
*
*number of segments participating in enclosure model (<= 8)
*flag to turn enclosure model on(=1) or off(=0)
*and gas participation (0=no, 1=yes)
4 1 0
*segment numbers for each participating segment
1 2 3 4
*inner(=-1) or outer(=1) for each segment
-1 -1 -1 -1
*emissivity of each surface
0.2 0.2 0.2 0.2
*area of each surface
297. 666. 281. 338.
*next n lines are the view factor matrix:
*view factor from 1 to 1, 1 to 2, etc. across
*view factor from 1 to 1, 2 to 1, etc. down
0.0064 0.7339 0.1766 0.0803
0.3255 0.3681 0.2367 0.0681
0.1867 0.5643 0.1872 0.0602
0.0746 0.1427 0.0529 0.7278
*next n lines are the path length matrix:
*path length from 1 to 1, 1 to 2, etc. across
*path length from 1 to 1, 2 to 1, etc. down
5.0 5.0 5.0 5.0
5.0 5.0 5.0 5.0
5.0 5.0 5.0 5.0
5.0 5.0 5.0 5.0
*first line contains number of user defined materials (1 <= n <= 10)
*next n lines contains user defined material properties
*specific heat, density, thermal conductivity and emissivity
*note: user defined material indices range from 20 to 29
2
100. 1000. 100. 0.1
644.5 7965. 27.24 0.2
*next three lines contain material index and emissivity
*1 2 3 4 5 6 7 8 9 10 11 12 13
*ss be lio2 beo c w air stm li v pb incl cu
0.20 0.60 0.60 0.60 0.60 0.60 0.0 0.0 0.10 0.85 0.60 0.20 0.60
*next eight lines contains heat transfer mode index reference
*1-cond 2-cond+rad 3-cond+rad+conv 4-gap
*5-rad 6-pebble bed 7-conv+rad 8-foil model
*note: flag 8 requires additional input as described after region input
*9-cond+rad (rad heat transfer is line-of-sight
*between inner surface and outer surface of region
*10-gap cond+rad (user defined gap conductance parallel with rad)
*note: flags 4, 5, 7, 8 and 10 should be used only for boundary conditions
*
*number of segments in model (<=8)
4
*
*SEGMENT 1
*
*decay heat multiplier set 1
*time to switch multiplier from set 1 to set 2
*(set time equal to zero for set 1 only)

```

```

*decay heat multiplier set 2
1.0 0. 1.0
*left (inner) boundary condition flag
*0=insulated, -1=fixed temp or -2=heat flux
*boundary temperature or heat flux (always required)
*note: use flag 5 to indicate connection to other surfaces
*using radiation enclosure model as described above
0 293.
*right (outer) boundary condition flag
*0=insulated, -1=fixed temp or -2=heat flux
*boundary temperature or heat flux (always required)
*note: use flag 5 to indicate connection to other surfaces
*using radiation enclosure model as described above
-1 1250.
*starting radius
7.0
*effective height
6.75
*total number of regions
1
*** region input ***
*each region input consist of three or more lines
*first line contains region character string id
*the next line contains the following fields:
*1) gap thickness preceeding region,
*2) gap conductance
*3) region thickness
*4) number of nodes in region
*5) boundary heat transfer mode for inner node
*6) heat transfer mode for middle nodes
*7) boundary heat transfer mode for outer node
*8) initial surface temperatures for region
*9) conduction length multiplier for region
*10) number of region materials
*the next one or two lines contain the following fields:
*1) material id for each material
*2) volume for each material
*3) power fractions for each material
ob fw armor - region 1
1.e-6 1.e6 0.010 5 5 1 4 1260. 1250. 1.0 1
21 1. 1.
*next four lines contain info to define user defined temperature output
*first line contains the integer number of different regions (<=8)
*second line contains list of integers identifying each region
*third line contains the number of temperatures points per region (total <=24)
*fourth line contains integer identifiers for each node within a region
1
1
5
1 2 3 4 5
*number of regions to be boiled (<=8)
1
*beginning and ending regions for each boiling region set
*and on/off flag (0=off,1=on)
1 1 0
*temperature, pressure, relief valve area,
*heat transfer coefficient, internal blanket area,
*valve flow coefficient, blanket liquid mass and
*relative lower and upper pressure setpoint

```

```

423. 2.e6 1.e-2 1.0 100. 100. 2.5e5 1.05 1.1
*number of auxiliary regions to be cooled/heated (<=8)
1
*auxiliary cooling flags (1=on,0=off)
0
*time to toggle flags
1.e9
*use constant (=0) or variable (=1) type energy term
1
*beginning and ending regions to be cooled/heated for each region group
1 1
*nominal energy rate for each region group (W)
-2.25e6
*nominal rejection temps
373.
*nominal region temps
423.
*segment, region and node number for temperature
*to control foil collapse
4 1 1
*number of regions with foils in preceding gap (<=8)
1
*region numbers
1
*number of foils per region
15
*emissivity of each foil group
0.08
*temperature for collapse of foils
3773.0
*fraction of foils that collapse
0.7
*gas name (air=0,stm=1)
1
*oxidation flag (1=on,0=off) and number of surfaces
*(-1=inner surface, 1=outer surface, 0=both surfaces)
0 -1
*next line contains rate flag and multiplier
*rate flag (0=full density, 1=12% porous,
*rate flag 2=geometric mean of full and porous (Divertor),
*rate flag 3=full density below 773 K,
*rate flag 4=geometric mean above 873 K,
*rate flag 5=interpolated between 773 K and 873 K (First Wall)
*rate flag 6=user input multiplicative (M) and exponential (E)
*rate flag 7=constants; i.e.,  $M \times \exp(-E/T)$  where T = temperature
*rate flag (NOTE: flag 4 requires extra line for two constants)
*multiplier: multiply reaction rate regardless of porous flag option
0 1.0
*region to apply oxidation model
1
*next set of input specifies regions for decay heat integration
*number of region groups to input (<=8)
1
*beginning and ending region numbers
1 1
*
*decay heat transient data
*first line has three inputs:
*1) is the decay energy distribution type

```

*decay (0) assumes spatial decay between points and integrates
 *discrete (1) changes at entered points in stairstep fashion
 *2) is which region index to start as r=0
 *3) is which direction to increment decay spatial coordinate
 * 0=inner to outer, 1=outer to inner
 *rest of decay data is arranged as follows:
 *1) number of time points, number of space points
 *2) radii entered starting from first wall armor (r=0.0)
 *3) time value
 *4) decay heat values entered corresponding to each space point
 *(repeat 3 and 4 for each time point)

1 1 0

8 12

0.0 0.0020005 0.0090015 0.0100025 0.0630035 0.0730045 0.0880045

0.206 0.324 0.442 0.560 0.561

.000000E+00

.93200000E+05	.81000000E+06	.18700000E+06	.14800000E+06	.88000000E+05

.73000000E+05	.31592732E+05	.70896111E+04	.15658062E+04	.34666319E+03

.000001E-09	.000001E-09			

.600000E+03

.43300000E+02	.38400000E+06	.13600000E+06	.10700000E+06	.63600000E+05

.53000000E+05	.23080701E+05	.51546389E+04	.11397941E+04	.25447934E+03

.000001E-09	.000001E-09			

.360000E+04

.43300000E+02	.11000000E+06	.10700000E+06	.83500000E+05	.50000000E+05

.41500000E+05	.18169913E+05	.40444090E+04	.89998593E+03	.19864969E+03

.000001E-09	.000001E-09			

.360000E+05

.43300000E+02	.67700000E+05	.29200000E+05	.22500000E+05	.14500000E+05

.12300000E+05	.57619905E+04	.13703409E+04	.32162507E+03	.75305112E+02

.000001E-09	.000001E-09			

.864000E+05

.43300000E+02	.41000000E+05	.21100000E+05	.16200000E+05	.10700000E+05

.92000000E+04	.44360779E+04	.10705789E+04	.25673580E+03	.61023108E+02

.000001E-09	.000001E-09			

.864000E+06

.43200000E+02	.17000000E+05	.17600000E+05	.13400000E+05	.88500000E+04

.75500000E+04	.36339827E+04	.87866768E+03	.20877416E+03	.48948323E+02

.000001E-09	.000001E-09			

.259200E+07

.43100000E+02	.16600000E+05	.15200000E+05	.11400000E+05	.75400000E+04

.64500000E+04	.30937960E+04	.74544009E+03	.17915080E+03	.41807321E+02

.000001E-09	.000001E-09			

.864000E+07

.40900000E+02	.14400000E+05	.49500000E+04	.35600000E+04	.22400000E+04

.18900000E+04	.85611393E+03	.18239492E+03	.40767388E+02	.89457280E+01

.000001E-09	.000001E-09			

*

*SEGMENT 2

*

*decay heat multiplier set 1

*time to switch multiplier from set 1 to set 2

*(set time equal to zero for set 1 only)

*decay heat multiplier set 2

0.0 0. 0.0

*left (inner) boundary condition flag

*0=insulated, -1=fixed temp or -2=heat flux

*boundary temperature or heat flux (always required)

*note: use flag 5 to indicate convection to other surfaces


```

*using radiation enclosure model as described above
0 293.
*right (outer) boundary condition flag
*0=insulated, -1=fixed temp or -2=heat flux
*boundary temperature or heat flux(always required)
*note: use flag 5 to indicate connection to other surfaces
*using radiation enclosure model as described above
-1 1250.
*starting radius
10.0
*effective height
10.6
*total number of regions
1
*** region input ***
*each region input consist of three or more lines
*first line contains region character string id
*the next line contains the following fields:
*1) gap thickness preceeding region,
*2) gap conductance
*3) region thickness
*4) number of nodes in region
*5) boundary heat transfer mode for inner node
*6) heat transfer mode for middle nodes
*7) boundary heat transfer mode for outer node
*8) initial surface temperatures for region
*9) conduction length multiplier for region
*10) number of region materials
*the next one or two lines contain the following fields:
*1) material id for each material
*2) volume for each material
*3) power fractions for each material
ob fw armor - region 1
1.e-6 1.e6 0.010 5 5 1 4 1260. 1250. 1.0 1
1 1. 1.
*next four lines contain info to define user defined temperature output
*first line contains the integer number of different regions (<=8)
*second line contains list of integers identifying each region
*third line contains the number of temperatures points per region (total <=24)
*fourth line contains integer identifiers for each node within a region
1
1
5
1 2 3 4 5
*number of regions to be boiled (<=8)
1
*beginning and ending regions for each boiling region set
*and on/off flag (0=off,1=on)
1 1 0
*temperature, pressure, relief valve area,
*heat transfer coefficient, internal blanket area,
*valve flow coefficient, blanket liquid mass and
*relative lower and upper pressure setpoint
423. 2.e6 1.e-2 1.0 100. 100. 2.5e5 1.05 1.1
*number of auxiliary regions to be cooled/heated (<=8)
1
*auxiliary cooling flags (1=on,0=off)
0
*time to toggle flags

```

```

1.e9
*use constant (=0) or variable (=1) type energy term
1
*beginning and ending regions to be cooled/heated for each region group
1 1
*nominal energy rate for each region group (W)
-2.25e6
*nominal rejection temps
373.
*nominal region temps
423.
*segment, region and node number for temperature
*to control foil collapse
1 1 1
*number of regions with foils in preceding gap (<=8)
1
*region numbers
1
*number of foils per region
15
*emissivity of each foil group
0.08
*temperature for collapse of foils
3773.0
*fraction of foils that collapse
0.7
*gas name (air=0,stm=1)
1
*oxidation flag (1=on,0=off) and number of surfaces
*(-1=inner surface, 1=outer surface, 0=both surfaces)
0 -1
*next line contains rate flag and multiplier
*rate flag (0=full density, 1=12% porous,
*rate flag 2=geometric mean of full and porous (Divertor),
*rate flag 3=full density below 773 K,
*rate flag 4=geometric mean above 873 K,
*rate flag 5=interpolated between 773 K and 873 K (First Wall)
*rate flag 6=user input multiplicative (M) and exponential (E)
*rate flag 7=constants; i.e.,  $M \times \exp(-E/T)$  where T = temperature
*rate flag 8=(NOTE: flag 4 requires extra line for two constants)
*multiplier: multiply reaction rate regardless of porous flag option
0 1.0
*region to apply oxidation model
1
*next set of input specifies regions for decay heat integration
*number of region groups to input (<=8)
1
*beginning and ending region numbers
1 1
*
*decay heat transient data
*first line has three inputs:
*1) is the decay energy distribution type
*decay (0) assumes spatial decay between points and integrates
*discrete (1) changes at entered points in stairstep fashion
*2) is which region index to start as r=0
*3) is which direction to increment decay spatial coordinate
* 0=inner to outer, 1=outer to inner
*rest of decay data is arranged as follows:

```

*1) number of time points, number of space points
 *2) radii entered starting from first wall armor (r=0.0)
 *3) time value
 *4) decay heat values entered corresponding to each space point
 *(repeat 3 and 4 for each time point)

1 1 0

8 12

0.0 0.0020005 0.0090015 0.0100025 0.0630035 0.0730045 0.0880045

0.206 0.324 0.442 0.560 0.561

.000000E+00

.93200000E+05 .81000000E+06 .18700000E+06 .14800000E+06 .88000000E+05

.73000000E+05 .31592732E+05 .70896111E+04 .15658062E+04 .34666319E+03

.000001E-09 .000001E-09

.600000E+03

.43300000E+02 .38400000E+06 .13600000E+06 .10700000E+06 .63600000E+05

.53000000E+05 .23080701E+05 .51546389E+04 .11397941E+04 .25447934E+03

.000001E-09 .000001E-09

.360000E+04

.43300000E+02 .11000000E+06 .10700000E+06 .83500000E+05 .50000000E+05

.41500000E+05 .18169913E+05 .40444090E+04 .89998593E+03 .19864969E+03

.000001E-09 .000001E-09

.360000E+05

.43300000E+02 .67700000E+05 .29200000E+05 .22500000E+05 .14500000E+05

.12300000E+05 .57619905E+04 .13703409E+04 .32162507E+03 .75305112E+02

.000001E-09 .000001E-09

.864000E+05

.43300000E+02 .41000000E+05 .21100000E+05 .16200000E+05 .10700000E+05

.92000000E+04 .44360779E+04 .10705789E+04 .25673580E+03 .61023108E+02

.000001E-09 .000001E-09

.864000E+06

.43200000E+02 .17000000E+05 .17600000E+05 .13400000E+05 .88500000E+04

.75500000E+04 .36339827E+04 .87866768E+03 .20877416E+03 .48948323E+02

.000001E-09 .000001E-09

.259200E+07

.43100000E+02 .16600000E+05 .15200000E+05 .11400000E+05 .75400000E+04

.64500000E+04 .30937960E+04 .74544009E+03 .17915080E+03 .41807321E+02

.000001E-09 .000001E-09

.864000E+07

.40900000E+02 .14400000E+05 .49500000E+04 .35600000E+04 .22400000E+04

.18900000E+04 .85611393E+03 .18239492E+03 .40767388E+02 .89457280E+01

.000001E-09 .000001E-09

*

*SEGMENT 3

*

*decay heat multiplier set 1

*time to switch multiplier from set 1 to set 2

*(set time equal to zero for set 1 only)

*decay heat multiplier set 2

0.0 0. 0.0

*left (inner) boundary condition flag

*0=insulated, -1=fixed temp or -2=heat flux

*boundary temperature or heat flux (always required)

*note: use flag 5 to indicate connection to other surfaces

*using radiation enclosure model as described above

0 293.

*right (outer) boundary condition flag

*0=insulated, -1=fixed temp or -2=heat flux

*boundary temperature or heat flux (always required)

*note: use flag 5 to indicate connection to other surfaces

```

*using radiation enclosure model as described above
-1 1250.
*starting radius
7.0
*effective height
6.4
*total number of regions
1
*** region input ***
*each region input consist of three or more lines
*first line contains region character string id
*the next line contains the following fields:
*1) gap thickness preceeding region,
*2) gap conductance
*3) region thickness
*4) number of nodes in region
*5) boundary heat transfer mode for inner node
*6) heat transfer mode for middle nodes
*7) boundary heat transfer mode for outer node
*8) initial surface temperatures for region
*9) conduction length multiplier for region
*10) number of region materials
*the next one or two lines contain the following fields:
*1) material id for each material
*2) volume for each material
*3) power fractions for each material
ob fw armor -          region 1
1.e-6 1.e6 0.010  5  5 1 4 1260. 1250.  1.0 1
1 1. 1.
*next four lines contain info to define user defined temperature output
*first line contains the integer number of different regions (<=8)
*second line contains list of integers identifying each region
*third line contains the number of temperatures points per region (total <=24)
*fourth line contains integer identifiers for each node within a region
1
1
5
1 2 3 4 5
*number of regions to be boiled (<=8)
1
*beginning and ending regions for each boiling region set
*and on/off flag (0=off,1=on)
1 1 0
*temperature, pressure, relief valve area,
*heat transfer coefficient, internal blanket area,
*valve flow coefficient, blanket liquid mass and
*relative lower and upper pressure setpoint
423. 2.e6 1.e-2 1.0 100. 100. 2.5e5 1.05 1.1
*number of auxiliary regions to be cooled/heated (<=8)
1
*auxiliary cooling flags (1=on,0=off)
0
*time to toggle flags
1.e9
*use constant (=0) or variable (=1) type energy term
1
*beginning and ending regions to be cooled/heated for each region group
1 1
*nominal energy rate for each region group (W)

```

```

-2.25e6
*nominal rejection temps
373.
*nominal region temps
423.
*segment, region and node number for temperature
*to control foil collapse
4 1 1
*number of regions with foils in preceding gap (<=8)
1
*region numbers
1
*number of foils per region
15
*emissivity of each foil group
0.08
*temperature for collapse of foils
3773.0
*fraction of foils that collapse
0.7
*gas name (air=0,stm=1)
1
*oxidation flag (1=on,0=off) and number of surfaces
*(-1=inner surface, 1=outer surface, 0=both surfaces)
0 -1
*next line contains rate flag and multiplier
*rate flag (0=full density, 1=12% porous,
*rate flag 2=geometric mean of full and porous (Divertor),
*rate flag 3=full density below 773 K,
*rate flag 4=geometric mean above 873 K,
*rate flag 5=interpolated between 773 K and 873 K (First Wall)
*rate flag 6=user input multiplicative (M) and exponential (E)
*rate flag 7=constants; i.e.,  $M \times \exp(-E/T)$  where T = temperature
*rate flag (NOTE: flag 4 requires extra line for two constants)
*multiplier: multiply reaction rate regardless of porous flag option
0 1.0
*region to apply oxidation model
1
*next set of input specifies regions for decay heat integration
*number of region groups to input (<=8)
1
*beginning and ending region numbers
1 1
*
*decay heat transient data
*first line has three inputs:
*1) is the decay energy distribution type
*decay (0) assumes spatial decay between points and integrates
*discrete (1) changes at entered points in stairstep fashion
*2) is which region index to start as r=0
*3) is which direction to increment decay spatial coordinate
* 0=inner to outer, 1=outer to inner
*rest of decay data is arranged as follows:
*1) number of time points, number of space points
*2) radii entered starting from first wall armor (r=0.0)
*3) time value
*4) decay heat values entered corresponding to each space point
*(repeat 3 and 4 for each time point)
1 1 0

```

8 12

0.0 0.0020005 0.0090015 0.0100025 0.0630035 0.0730045 0.0880045

0.206 0.324 0.442 0.560 0.561

.000000E+00

.93200000E+05 .81000000E+06 .18700000E+06 .14800000E+06 .88000000E+05

.73000000E+05 .31592732E+05 .70896111E+04 .15658062E+04 .34666319E+03

.000001E-09 .000001E-09

.600000E+03

.43300000E+02 .38400000E+06 .13600000E+06 .10700000E+06 .63600000E+05

.53000000E+05 .23080701E+05 .51546389E+04 .11397941E+04 .25447934E+03

.000001E-09 .000001E-09

.360000E+04

.43300000E+02 .11000000E+06 .10700000E+06 .83500000E+05 .50000000E+05

.41500000E+05 .18169913E+05 .40444090E+04 .89998593E+03 .19864969E+03

.000001E-09 .000001E-09

.360000E+05

.43300000E+02 .67700000E+05 .29200000E+05 .22500000E+05 .14500000E+05

.12300000E+05 .57619905E+04 .13703409E+04 .32162507E+03 .75305112E+02

.000001E-09 .000001E-09

.864000E+05

.43300000E+02 .41000000E+05 .21100000E+05 .16200000E+05 .10700000E+05

.92000000E+04 .44360779E+04 .10705789E+04 .25673580E+03 .61023108E+02

.000001E-09 .000001E-09

.864000E+06

.43200000E+02 .17000000E+05 .17600000E+05 .13400000E+05 .88500000E+04

.75500000E+04 .36339827E+04 .87866768E+03 .20877416E+03 .48948323E+02

.000001E-09 .000001E-09

.259200E+07

.43100000E+02 .16600000E+05 .15200000E+05 .11400000E+05 .75400000E+04

.64500000E+04 .30937960E+04 .74544009E+03 .17915080E+03 .41807321E+02

.000001E-09 .000001E-09

.864000E+07

.40900000E+02 .14400000E+05 .49500000E+04 .35600000E+04 .22400000E+04

.18900000E+04 .85611393E+03 .18239492E+03 .40767388E+02 .89457280E+01

.000001E-09 .000001E-09

*

*SEGMENT 4

*

*decay heat multiplier set 1

*time to switch multiplier from set 1 to set 2

*(set time equal to zero for set 1 only)

*decay heat multiplier set 2

0.0 0. 0.0

*left (inner) boundary condition flag

*0=insulated, -1=fixed temp or -2=heat flux

*boundary temperature or heat flux (always required)

*note: use flag 5 to indicate connection to other surfaces

*using radiation enclosure model as described above

0 293.

*right (outer) boundary condition flag

*0=insulated, -1=fixed temp or -2=heat flux

*boundary temperature or heat flux (always required)

*note: use flag 5 to indicate connection to other surfaces

*using radiation enclosure model as described above

-1 446.

*starting radius

7.0

*effective height

7.7

```

*total number of regions
1
*** region input ***
*each region input consist of three or more lines
*first line contains region character string id
*the next line contains the following fields:
*1) gap thickness preceeding region,
*2) gap conductance
*3) region thickness
*4) number of nodes in region
*5) boundary heat transfer mode for inner node
*6) heat transfer mode for middle nodes
*7) boundary heat transfer mode for outer node
*8) initial surface temperatures for region
*9) conduction length multiplier for region
*10) number of region materials
*the next one or two lines contain the following fields:
*1) material id for each material
*2) volume for each material
*3) power fractions for each material
ob fw armor - region 1
1.e-6 1.e6 0.010 5 5 1 4 456. 446. 1.0 1
1 1. 1.
*next four lines contain info to define user defined temperature output
*first line contains the integer number of different regions (<=8)
*second line contains list of integers identifying each region
*third line contains the number of temperatures points per region (total <=24)
*fourth line contains integer identifiers for each node within a region
1
1
5
1 2 3 4 5
*number of regions to be boiled (<=8)
1
*beginning and ending regions for each boiling region set
*and on/off flag (0=off,1=on)
1 1 0
*temperature, pressure, relief valve area,
*heat transfer coefficient, internal blanket area,
*valve flow coefficient, blanket liquid mass and
*relative lower and upper pressure setpoint
423. 2.e6 1.e-2 1.0 100. 100. 2.5e5 1.05 1.1
*number of auxiliary regions to be cooled/heated (<=8)
1
*auxiliary cooling flags (1=on,0=off)
0
*time to toggle flags
1.e9
*use constant (=0) or variable (=1) type energy term
1
*beginning and ending regions to be cooled/heated for each region group
1 1
*nominal energy rate for each region group (W)
-2.25e6
*nominal rejection temps
373.
*nominal region temps
423.
*segment, region and node number for temperature

```

```

*to control foil collapse
1 1 1
*number of regions with foils in preceding gap (<=8)
1
*region numbers
1
*number of foils per region
15
*emissivity of each foil group
0.08
*temperature for collapse of foils
3773.0
*fraction of foils that collapse
0.7
*gas name (air=0,stm=1)
1
*oxidation flag (1=on,0=off) and number of surfaces
*(-1=inner surface, 1=outer surface, 0=both surfaces)
0 -1
*next line contains rate flag and multiplier
*rate flag (0=full density, 1=12% porous,
*rate flag 2=geometric mean of full and porous (Divertor),
*rate flag 3=full density below 773 K,
*rate flag 4=geometric mean above 873 K,
*rate flag 5=interpolated between 773 K and 873 K (First Wall)
*rate flag 6=user input multiplicative (M) and exponential (E)
*rate flag 7=constants; i.e.,  $M \times \exp(-E/T)$  where T = temperature
*rate flag 8 (NOTE: flag 4 requires extra line for two constants)
*multiplier: multiply reaction rate regardless of porous flag option
0 1.0
*region to apply oxidation model
1
*next set of input specifies regions for decay heat integration
*number of region groups to input (<=8)
1
*beginning and ending region numbers
1 1
*
*decay heat transient data
*first line has three inputs:
*1) is the decay energy distribution type
*decay (0) assumes spatial decay between points and integrates
*discrete (1) changes at entered points in stairstep fashion
*2) is which region index to start as r=0
*3) is which direction to increment decay spatial coordinate
* 0=inner to outer, 1=outer to inner
*rest of decay data is arranged as follows:
*1) number of time points, number of space points
*2) radii entered starting from first wall armor (r=0.0)
*3) time value
*4) decay heat values entered corresponding to each space point
*(repeat 3 and 4 for each time point)
1 1 0
8 12
0.0 0.0020005 0.0090015 0.0100025 0.0630035 0.0730045 0.0880045
0.206 0.324 0.442 0.560 0.561
.000000E+00
.93200000E+05 .81000000E+06 .18700000E+06 .14800000E+06 .88000000E+05
.73000000E+05 .31592732E+05 .70896111E+04 .15658062E+04 .34666319E+03

```


.000001E-09	.000001E-09			
.600000E+03				
.43300000E+02	.38400000E+06	.13600000E+06	.10700000E+06	.63600000E+05
.53000000E+05	.23080701E+05	.51546389E+04	.11397941E+04	.25447934E+03
.000001E-09	.000001E-09			
.360000E+04				
.43300000E+02	.11000000E+06	.10700000E+06	.83500000E+05	.50000000E+05
.41500000E+05	.18169913E+05	.40444090E+04	.89998593E+03	.19864969E+03
.000001E-09	.000001E-09			
.360000E+05				
.43300000E+02	.67700000E+05	.29200000E+05	.22500000E+05	.14500000E+05
.12300000E+05	.57619905E+04	.13703409E+04	.32162507E+03	.75305112E+02
.000001E-09	.000001E-09			
.864000E+05				
.43300000E+02	.41000000E+05	.21100000E+05	.16200000E+05	.10700000E+05
.92000000E+04	.44360779E+04	.10705789E+04	.25673580E+03	.61023108E+02
.000001E-09	.000001E-09			
.864000E+06				
.43200000E+02	.17000000E+05	.17600000E+05	.13400000E+05	.88500000E+04
.75500000E+04	.36339827E+04	.87866768E+03	.20877416E+03	.48948323E+02
.000001E-09	.000001E-09			
.259200E+07				
.43100000E+02	.16600000E+05	.15200000E+05	.11400000E+05	.75400000E+04
.64500000E+04	.30937960E+04	.74544009E+03	.17915080E+03	.41807321E+02
.000001E-09	.000001E-09			
.864000E+07				
.40900000E+02	.14400000E+05	.49500000E+04	.35600000E+04	.22400000E+04
.18900000E+04	.85611393E+03	.18239492E+03	.40767388E+02	.89457280E+01
.000001E-09	.000001E-09			