CHEMCON User's Manual

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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. The code includes properties for 13 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 ITER reactor design 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. Section 2 describes the oxidation reactions for steam and air with graphite, beryllium, 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 ITER and gives a detailed description of the input format. Section 5 contains a list of References. Finally, Appendix A contains the thermal properties table, Appendix B contains a listing of 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:

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

where

ρ	=	density (kg/m ³)
C_p	=	specific heat (J/kg · K)
T	=	temperature (K)
t	=	time (s)
r	=	major radius (m)
k	=	thermal conductivity (W/m · K)
q	=	heat rate density (W/m ³).

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 follows an exponential form:

$$q = q_0 e^{-B(r-r_0)} \quad (3)$$

and where B and r_0 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.

Performing the integration and using standard finite difference representations, Equation (2) becomes:

$$\begin{aligned}
& \frac{(r_{i+1/2}^2 - r_{i-1/2}^2)}{2} \rho C_p \frac{(T_i^{n+1} - T_i^n)}{t^{n+1} - t^n} \\
&= r_{i+1/2} k_{i+1/2} \frac{T_{i+1}^{n+1} - T_i^{n+1}}{r_{i+1} - r_i} - r_{i-1/2} k_{i-1/2} \frac{T_i^{n+1} - T_{i-1}^{n+1}}{r_i - r_{i-1}} \\
&+ \frac{q_o e^{-B(r_{i+1/2} - r_o)}}{B^2} (Br_{i+1/2} - 1) - \frac{q_o e^{-B(r_{i-1/2} - r_o)}}{B^2} (Br_{i-1/2} - 1)
\end{aligned} \tag{4}$$

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

Equation 4 can be expressed in more compact notation as:

$$V_i \rho C_p \frac{(T_i^{n+1} - T_i^n)}{t^{n+1} - t^n} = G_{i+1/2} (T_{i+1}^{n+1} - T_i^{n+1}) - G_{i-1/2} (T_i^{n+1} - T_{i-1}^{n+1}) + V_i \bar{q}_i \tag{5}$$

where

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

V_i = zone volume (m^3).

Also, $\bar{q}_i$ is simply a compact representation of the last two terms in Equation (4).

The thermal conductance of Equation 5 is defined as

$$G_{i+1/2} = 2\pi L \left(\frac{r_{i+1/2} k_{i+1/2}}{r_{i+1} - r_i} \right) \text{ and } G_{i-1/2} = 2\pi L \left(\frac{r_{i-1/2} k_{i-1/2}}{r_i - r_{i-1}} \right) \tag{6}$$

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

$$V_i = \pi L (r_{i+1/2}^2 - r_{i-1/2}^2). \tag{7}$$

The thermal conductance expressions for pure conduction have been described. The next section describes the conductance forms for the other heat transfer modes used in the CHEMCON code.

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

$$G_{i+1/2} = 2\pi L r_{i+1/2} h_{i+1/2} \quad (8)$$

where h_i is a generic heat transfer coefficient ($\text{W}/\text{m}^2 \cdot \text{K}$). 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 as

$$h_{\text{rad}} = \sigma \epsilon_{\text{eff}} (T_{i+1}^2 + T_i^2) (T_{i+1} + T_i) \quad (9)$$

where

σ = Stefan-Boltzmann constant

ϵ_{eff} = effective emissivity

and where the effective emissivity between the surfaces is

$$\epsilon_{\text{eff}} = \left[\frac{1}{\epsilon_i} + \frac{r_i}{r_{i+1}} \left(\frac{1}{\epsilon_{i+1}} - 1 \right) \right]^{-1} \quad (10)$$

The following correlations are used for natural convective heat transfer:²

$$Nu_{\delta} = 0.180 Gr_{\delta}^{1/4} \left(\frac{\delta}{L} \right)^{1/9} \text{ for } Gr_{\delta} < 20,000 \quad (11)$$

and

$$Nu_{\delta} = 0.065 Gr_{\delta}^{1/3} \left(\frac{\delta}{L} \right)^{1/9} \text{ for } Gr_{\delta} > 20,000. \quad (12)$$

These correlations are for natural convection between two vertical surfaces of an enclosure.

For conduction through a packed pebble bed, the effective thermal conductivity is predicted by the model proposed by Hall and Martin³ which is as follows:

$$k_{\text{eff}} = \frac{P_f k_g}{0.524} \left[\frac{(\pi/2)(1-\lambda)}{\delta(1-\lambda)-1} - \frac{(\pi/2)(1+m)}{[\delta(1-\lambda)-1]^2} \ln \frac{\delta(1+\lambda m)+m}{(1+\lambda \delta)(1+m)} + (1-\pi/4)(1+\lambda) \right] \quad (13)$$

where

k_b = pebble conductivity ($\text{W}/\text{m} \cdot \text{K}$)

k_g	=	gas conductivity (W/m · K)
T	=	temperature (K)
δ	=	k_g/k_b
D_p	=	pebble diameter (m x 10 ⁻⁶)
m	=	$3.0833 \times 10^{-4} T^{1.168} / (P_g D_p)$
P_f	=	packing fraction
P_g	=	gas pressure (Pa x 10 ⁶)
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:

$$G_{i+1/2} = 2\pi L r_{i+1/2} \sum_j C_j h_j. \quad (14)$$

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.

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.

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.

2. OXIDATION REACTIONS

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

2.1 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 these two reactions proceed was measured for various graphites and reported in Reference 4. 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:

$$R_{ox} = 8.54 \times 10^7 e^{-70,800/RT} \quad (17)$$

for temperatures less than 1460 K, and

$$R_{ox} = 5.18 e^{-22,500/RT} \quad (18)$$

for temperatures between 1460 K and 2000 K (R is the Universal Gas Constant, equal $1.987 \text{ cal/g-mole} \cdot \text{K}$).

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:

$$R_{ox} = 0.12 e^{-11,300/RT} \quad (19)$$

for temperatures less than 1273 K, and

$$R_{ox} = 0.0076 e^{-4475/RT} \quad (20)$$

for temperatures between 1273 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 (17-20). Temperature dependent heats of formation were obtained from Reference 6. The heat of formation for carbon monoxide (J/kg-CO) is:

$$h_{f_{co}} = -\frac{4187}{M_{co}} \left(25400 + 0.89T + 0.00027T^2 + 219000T^{-1} \right) \quad (21)$$

for carbon dioxide (J/kg-CO₂) is:

$$h_{f_{co_2}} = -\frac{4187}{M_{co_2}} \left(93690 + 0.71T + 0.00007T^2 + 46000T^{-1} \right) \quad (22)$$

and for water (J/kg-H₂O) is:

$$h_{f_{h_2o}} = -\frac{4187}{M_{H_2O}} \left(56930 + 2.93T + (-0.00064)T^2 + 16000T^{-1} \right) \quad (23)$$

The rate at which energy is consumed (W/m²) then is:

$$q_{ox} = - \left(h_{f_{co}} - h_{f_{h_2o}} \frac{M_{H_2O}}{M_{CO}} \right) \left(\frac{M_{CO}}{M_C} \right) R_{ox} \quad (24)$$

where M_{CO}, M_{H₂O}, M_C are the molecular weights of carbon monoxide, water, and carbon, respectively.

The rate at which energy is produced (W/m²) then is:

$$q_{ox} = - (h_{f_{co}}) \left(\frac{M_{CO}}{M_C} \right) R_{ox} \quad (25)$$

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

2.2 Beryllium Oxidation

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

The rate at which this reaction proceeds was measured and reported in Reference 4. The Arrhenius type oxidation rate relationships (kg-beryllium/m² · s) developed from these measurements for full density beryllium are as follows:

$$R_{ox} = 1.933 \times 10^6 e^{-51,180/RT} \quad (27)$$

for temperatures less than 1173 K, and

$$R_{ox} = 31.84 e^{-25,400/RT} \quad (28)$$

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

$$R_{ox} = 49.471 e^{-12,500/T} \quad (29)$$

The beryllium-water oxidation reaction is 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 (27-29). Temperature dependent heats of formation were obtained from Reference 5. For beryllium oxide the heat of formation (J/kg-BeO) is:

$$h_{f_{co}} = \frac{4187}{M_{BeO}} \left(-144,220 + 0.83T + 0.00046T^2 + 248,000T^{-1} \right) \quad (30)$$

and for water (J/kg-H₂O) as given by Equation (23).

The rate at which energy is released (W/m²) then is:

$$q_{ox} = - \left(h_{f_{BeO}} - h_{f_{H_2O}} \frac{M_{H_2O}}{M_{BeO}} \right) \left(\frac{M_{BeO}}{M_{Be}} \right) R_{ox} \quad (31)$$

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

2.3 Tungsten Oxidation

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

The rate at which this reaction proceeds was measured and reported in Reference 5. The Arrhenius type oxidation rate relationships (kg-tungsten/m² · s) developed from these measurements is as follows:

$$R_{ox} = 136 e^{-30,890/RT} \quad (33)$$

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 Equation (33). Temperature dependent heats of formation were obtained from Reference 6. For tungsten oxide the heat of formation (J/kg-WO₃) is:

$$h_{f_{WO_3}} = \frac{4187}{M_{WO_3}} \left(-201,180 + 1.27T + 0.00181T^2 - 60,000T^{-1} \right) \quad (34)$$

and for water (J/kg-H₂O) as given by Equation (23).

The rate at which energy is released (W/m²) is then:

$$q_{ox} = - \left(h_{f_{WO_3}} - h_{f_{H_2O}} \frac{3M_{H_2O}}{M_{WO_3}} \right) \left(\frac{M_{WO_3}}{M_W} \right) R_{ox} \quad (35)$$

where M_{WO₃}, M_{H₂O}, M_W are the molecular weights of tungsten oxide, water, 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. Appendix A contains the equations for these material properties in the CHEMCON code. Air and water properties are obtained from tables as given in Appendix B.

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 heat into and out of the cell defined at the physical cell boundaries and energy generation due to decay heat or chemical reactions (Equation 4). 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. 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, we suggest using a large gap conductance (i.e., $> 10^6$ (W/m² K)) and a very small (10^{-6} m) gap to match actual geometry. This effectively gives the two region surfaces the same temperature.

Generally, the input sequence contains general model information (e.g. transient time, vacuum vessel cooling on or off, etc.) followed by detailed nodal information (thickness, initial temperature, etc.) and finally transient spatial decay heat information. Distance is input in meters (m), temperature in Kelvin (K), and power in watts (W).

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 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.

**decay heat multipliers (inboard and outboard)*
1.0 1.0

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.

**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*
0.30 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 two lines contains heat transfer mode index*
**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 general region input*
**note: flags 4, 5, 7 and 8 should be used only for boundary conditions*

The next input group specifies the starting radius for the problem geometry.

**starting radius*
1.e-6

The next input group specifies the effective height for the problem geometry.

**effective height*
11.72

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

**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 preceding 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 temperature for region
 *9) 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
 1 1. 1.
ib solenoid - region 2
 1.e-6 1.e6 0.815 2 4 1 4 4.5 1
 1 1. 1.
ib tf magnet - region 3
 1.e-6 1.e6 0.895 2 4 1 8 4.5 1
 1 1. 1.
ib tf foils outer - region 4
 0.065 3.e3 0.0005 2 8 1 8 77. 1
 1 1. 1.
ib gamma shield - region 5
 0.065 3.e3 0.030 2 8 1 4 77. 1
 11 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 user selected regions (≤ 12)
 *second line contains list of integers identifying each region
 *third line contains the number of temperatures points per region to be output (total ≤ 24)
 *fourth line contains integer identifiers for the node temperatures within a region to be output
 6
 3 5 48 50 51 53
 2 2 2 2 2 2
 1 2 1 2 1 2 1 2 1 2

The next input group consists of region locations for vacuum vessel. The temperature of the vacuum vessel is used for the foil collapse model.

*beginning and ending regions for inboard vacuum vessel
 6 8
 *beginning and ending regions for outboard vacuum vessel
 45 47

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.

**number of auxiliary cooled/heated region groups (≤ 12)*
5
**auxiliary cooling flags (1=on,0=off)*
1 1 1 1 1
**beginning and ending regions to be cooled/heated for each region group*
6 8
45 47
4 4
49 49
52 52
**nominal power for each region group (W)*
-0.75e6 -2.25e6 -8.e3 -24.e3 -5.e3
**nominal rejection temps*
423. 423. 70. 70. 70.
**nominal region temps*
473. 473. 77. 77. 77.

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-by-one 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.

**number of regions with foils in adjacent gap (≤ 12)*
6
**region numbers*
4 5 49 50 52 53
**number of foils preceding region*
15 30 30 15 15 30
**emissivity of each foil group*
0.3 0.3 0.3 0.3 0.3 0.3
**temperature for collapse of foils*

773.0 773.0 773.0 773.0 3773.0 3773.0

**fraction of foil area that collapses*

0.7 0.7 0.7 0.7 0.7 0.7

The next input group consists of oxidation model information.

**gas name (air or stm)*

stm

**oxidation flag (1=on,0=off) and number of surfaces (1 or 2)*

1 1

**porous flag (1=porous, 0=full density) for armor (be only)*

0

**beginning and ending regions for inboard armor*

26 26

**beginning and ending regions for outboard armor*

27 27

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 (<= 12)*

9

**beginning and ending region numbers*

26 26

27 27

25 25

28 28

21 25

28 32

9 20

33 44

1 54

The next input group contains transient decay heat data. The zero radius for the spatial decay heat points coincides with the last node of the inboard first wall armor and decays as the model radius decreases and with the first node of the outboard first wall armor and decays as the model radius increases. There are two sets of input: the first for the inboard and the second for the outboard.

**decay heat transient data*

**first line is type of input:*

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

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

**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

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

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.

There are two temperature output files produced: **user.temps** and **iter.3dout**. **user.temps** contains the user defined temperatures. **iter.3dout** contains the temperatures at each node location through time.

The **itereda.out** output file contains the decay heat accounting done by CHEMCON for each radial cell through time. The output file **iter.udec** contains the user defined decay heat output. The output file **iter.ueng** contains the user defined integrated decay heat output. Finally, the output file **itereda.gas** contains the amount of hydrogen or carbon dioxide produced during the transient.

5.0 REFERENCES

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Appendix A

Temperature Dependent Material Property Tables

Material Property Table.^{6,8,9}

Material	Density (kg/m^3)	Specific Heat ($\text{J/kg} \cdot \text{K}$)	Thermal Conductivity ($\text{W/m} \cdot \text{k}$)	Emissivity
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 $300 < T < 1395 \text{ K}$; $285.19 \cdot \log(T) - 238.52$, 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 $400 < T < 2000 \text{ K}$	$(1-P) 42.17 10^4 [\log(T) (1.81570.5997 \log(T))]$ 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	1358.0	$353.17 + 0.117 T$, for $323 < T < 1273 \text{ K}$	320.0, for $166 < T < 1356 \text{ K}$	0.6

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

*total transient time in days
 100.0
 *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. 120.0 360
 1.93e9 180.0 1440
 1.96e9 180.0 1440
 *decay heat multipliers (inboard and outboard)
 1.0 1.0
 *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
 0.30 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 two lines contains heat transfer mode index
 *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 general region input
 *note: flags 4, 5, 7 and 8 should be used only for boundary conditions
 *starting radius
 1.e-6
 *effective height
 11.72
 *total number of regions
 54
 *** 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 temperature for region
 *9) 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
 1 1. 1.
 ib solenoid - region 2
 1.e-6 1.e6 0.815 2 4 1 4 4.5 1
 1 1. 1.
 ib tf magnet - region 3
 1.e-6 1.e6 0.895 2 4 1 8 4.5 1
 1 1. 1.
 ib tf foils outer - region 4
 0.065 3.e2 0.0005 2 8 1 8 77. 1
 1 1. 1.
 ib gamma shield - region 5

0.065 3.e2 0.030 2 8 1 4 77. 1
 11 1. 1.
 ib vv a - region 6
 1.e-6 1.e6 0.030 2 4 1 4 473. 1
 12 1. 1.
 ib vv b - region 7
 1.e-6 1.e6 0.400 10 4 6 4 473. 1
 1 0.80 1.
 ib vv c - region 8
 1.e-6 1.e6 0.030 2 4 1 5 473. 1
 12 1. 1.
 ib blanket a 1 - region 9
 0.05 1.e6 0.0861 2 5 1 4 523. 1
 1 1. 1.
 ib blanket a 2 - region 10
 1.e-6 1.e6 0.0159 2 4 2 4 523. 1
 1 0.1 1.
 ib blanket b 1 - region 11
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.90 1.
 ib blanket b 2 - region 12
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.25 1.
 ib blanket b 3 - region 13
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.90 1.
 ib blanket b 4 - region 14
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.25 1.
 ib blanket b 5 - region 15
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.90 1.
 ib blanket b 6 - region 16
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.25 1.
 ib blanket b 7 - region 17
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.90 1.
 ib blanket b 8 - region 18
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.25 1.
 ib blanket b 9 - region 19
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.90 1.
 ib blanket b 10 - region 20
 1.e-6 1.e6 0.0306 2 4 2 4 523. 1
 1 0.25 1.
 ib fw a - supports 1 - region 21
 1.e-6 1.e6 0.005 2 4 2 4 633. 1
 1 0.2 1.
 ib fw a - supports 2 - region 22
 1.e-6 1.e6 0.010 2 4 1 4 633. 1
 1 1.0 1.
 ib fw a - supports 3 - region 23
 1.e-6 1.e6 0.053 2 4 2 4 633. 1
 1 0.15 1.
 ib fw b - ss backing - region 24
 1.e-6 1.e6 0.001 2 4 1 4 633. 1
 1 1. 1.

ib fw b - cu - region 25
 1.e-6 1.e6 0.007 2 4 1 4 633. 1
 13 1. 1.
 ib fw armor - region 26
 1.e-6 1.e6 0.002 2 4 1 5 633. 1
 2 1. 1.
 ob fw armor - region 27
 6.617 1.e6 0.002 2 5 1 4 633. 1
 2 1. 1.
 ob fw b - cu - region 28
 1.e-6 1.e6 0.007 2 4 1 4 633. 1
 13 1. 1.
 ob fw b - ss backing - region 29
 1.e-6 1.e6 0.001 2 4 1 4 633. 1
 1 1. 1.
 ob fw a - supports 3 - region 30
 1.e-6 1.e6 0.053 2 4 2 4 633. 1
 1 0.10 1.
 ob fw a - supports 2 - region 31
 1.e-6 1.e6 0.010 2 4 1 4 633. 1
 1 1.0 1.
 ob fw a - supports 1 - region 32
 1.e-6 1.e6 0.015 2 4 2 4 633. 1
 1 0.2 1.
 ob blanket b 10 - region 33
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.30 1.
 ob blanket b 9 - region 34
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.95 1.
 ob blanket b 8 - region 35
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.30 1.
 ob blanket b 7 - region 36
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.95 1.
 ob blanket b 6 - region 37
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.30 1.
 ob blanket b 5 - region 38
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.95 1.
 ob blanket b 4 - region 39
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.30 1.
 ob blanket b 3 - region 40
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.95 1.
 ob blanket b 2 - region 41
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.30 1.
 ob blanket b 1 - region 42
 1.e-6 1.e6 0.0354 2 4 2 4 523. 1
 1 0.95 1.
 ob blanket a 2 - region 43
 1.e-6 1.e6 0.0301 2 4 2 4 523. 1
 1 0.1 1.
 ob blanket a 1 - region 44
 1.e-6 1.e6 0.0878 2 4 1 5 523. 1

```

1 1. 1.
ob vv c -                region 45
0.227 1.e6 0.040 2 5 1 4 473. 1
12 1. 1.
ob vv b -                region 46
1.e-6 1.e6 0.590 10 4 6 4 473. 1
1 0.80 1.
ob vv a -                region 47
1.e-6 1.e6 0.040 2 4 1 4 473. 1
12 1. 1.
ob gamma shield -       region 48
1.e-6 1.e6 0.030 2 4 1 8 77. 1
11 1. 1.
ob tf foils inner -     region 49
0.100 3.e2 0.0005 2 8 2 8 77. 1
1 1. 1.
ob tf magnet/strct a -  region 50
0.118 3.e2 1.118 2 8 2 5 4.5 1
1 1. 1.
ob tf magnet/strct b -  region 51
0.001 1.e6 1.04 2 5 2 8 4.5 1
1 1. 1.
ob tf foils outer -     region 52
1.32 3.e2 0.0005 2 8 2 8 77. 1
1 1. 1.
ob cryostat -           region 53
1.32 3.e2 2.0 2 8 1 4 77. 1
1 1. 1.
fixed temp sink -       region 54
1.e-6 1.e6 1.0 2 4 1 4 298. 1
1 1. 1.
*next four lines contain info to define user defined temperature output
*first line contains the integer number of different regions (<=12)
*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
6
3 5 48 50 51 53
2 2 2 2 2 2
1 2 1 2 1 2 1 2 1 2 1 2
*beginning and ending regions for inboard vacuum vessel
6 8
*beginning and ending regions for outboard vacuum vessel
45 47
*number of auxiliary regions to be cooled/heated (<=12)
5
*auxiliary cooling flags (1=on,0=off)
1 1 1 1 1
*beginning and ending regions to be cooled/heated for each region group
6 8
45 47
4 4
49 49
52 52
*nominal energy rate for each region group (W)
-0.75e6 -2.25e6 -8.e3 -24.e3 -5.e3
*nominal rejection temps
423. 423. 70. 70. 70.
*nominal region temps

```

473. 473. 77. 77. 77.
 *number of regions with foils in preceding gap (<=12)
 6
 *region numbers
 4 5 49 50 52 53
 *number of foils per region
 15 30 30 15 15 30
 *emissivity of each foil group
 0.08 0.08 0.08 0.08 0.08 0.08
 *temperature for collapse of foils
 3773.0 3773.0 3773.0 3773.0 3773.0 3773.0
 *fraction of foils that collapse
 0.7 0.7 0.7 0.7 0.7 0.7
 *gas name (air or stm)
 stm
 *oxidation flag (1=on,0=off) and number of surfaces (1 or 2)
 1 1
 *porous flag (1=porous,0=full density)
 0
 *beginning and ending regions for inboard armor
 26 26
 *beginning and ending regions for outboard armor
 27 27
 *next set of input specifies regions for decay heat integration
 *number of region groups to input (<=12)
 9
 *beginning and ending region numbers
 26 26
 27 27
 25 25
 28 28
 21 25
 28 32
 9 20
 33 44
 1 54
 *decay heat transient data
 *first line is type of input:
 *decay (0) assumes spatial decay between points and integrates
 *discrete (1) changes at entered points in stairstep fashion
 *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
 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
 .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			
8 12				
0.0 0.002005 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			