|  |  |
| --- | --- |
|  |  |
| PSI-Logo_narrow | Rooster-mf User’s Guide  Part-I: Input Manual  November 2024  Paul Scherrer Institute  Scientific Computing, Theory and Data  Laboratory for Simulation and Modelling  Advanced Nuclear Systems Group |

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# Introduction

The Rooster-mf code is under active development at PSI as an Open-Source code framework for simulation of Gen-IV Liquid Metal Fast Breeding Reactor system behaviour utilizing Fortran 95/2003 language, which supports parallel acceleration approach and object-oriented programming characteristics.

The input file for Rooster-mf code is arranged in a NAMELIST style. In this format, the input variables/arrays are divided into classes that correspond to different NAMELISTs, each class is distinguished by a different NAMELIST name. Within each NAMELIST, the input variables can be freely ordered, and between the NAMELISTs the comments can be arbitrarily typed since they are simply ignored.

The NAMELIST classes of the input stream of Rooster-mf code currently includes:

&XTIME: variables relative to calculation time/time-step control /

&XSOLV: flags for problem type, variables for settings of ode solver /

&XPIPE: variables for defining & setting fluid pipe object /

&XJUNC: variables for defining & setting fluid junction object /

&XCORE: variables for defining & setting core neutronics parameters /

&XFUEL: variables for defining & setting fuel pellet object /

&XCLAD: variables for defining & setting cladding object /

&XFROD: variables for defining & setting fuel-rod object /

&XTHBC: variables for defining & setting thermal boundary object /

&XHSTR: variables for defining & setting heat structure object /

&XSGNL: variables for defining & setting signal object /

The purpose of this document is to provide the users with necessary information about developing and editing input file before executing Rooster-mf code.

# XTIME

XTIME卡片主要包含算例的起止物理时间、结果输出时间步长、求解器的时间步长等控制变量，该卡片的设置对于计算效率和收敛性有明显影响。该卡片仅需输入一次，当一个input文件中出现多个XTIME卡时，程序仅读取最先出现的卡片数据。

## Descriptions of input variables

|  |  |  |  |
| --- | --- | --- | --- |
| **Variable** | **Type** | **Default** | **Description** |
| tstart | real(c\_doube) | 0.d+00 | (s) | |
| tend | real(c\_doube) | 1.d+02 | (s) | |
| dtout | real(c\_doube) | 1.d+01 | (s) | |
| dtini | real(c\_doube) | 1.d-08 | (s) | |
| dtmin | real(c\_doube) | 1.d-08 | (s) | |
| dtmax | real(c\_doube) | 1.d-01 | (s) | |

Specially, for users in PSI, FRED code should be installed in Merlin6 cluster. The detail of requesting the access to Merlin6 cluster is attached in Appendix A.

## Input examples

To install FRED, firstly putting the FRED source files in your system (for example, source files in path */user/FRED/00.FRED.SRC*), then you can enter the folder:

cd /user/FRED/00.FRED.SRC

In case, it is suggested to clear the object files (.o) generated at previous compilation:

rm \*.o

Then compile the source files:

chmod u+x compile

./compile

In this way, an executable file *fred.x* will be generated, which is used to run the FRED input deck.

## FRED input deck description

An input deck *fred* is necessary while running FRED, it defines the parameters of calculation case. The input deck consists of cards. Free format is used. Any card starting with \* is a comment card. Below is an example of the input deck and explanation of the cards, users can refer to the *Rinp.for* file for more detailed explanations.

\*

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* TIME INTEGRATION CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno meth rtol atol hmax

000000 GEAR0 1.0E-5 1.E-5 7200.

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* TRANSIENT CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno itran nout ntrac

000001 0 1 0

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* OPTION CARDS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

000002 OUTPUT\_AXIAL\_LAYER 4

000002 OUTPUT\_FUEL\_ROD 1

\*

000002 FGR

000002 FUEL\_CREEP

000002 FUEL\_SWEL

\*000002 FUEL\_PLAS

000002 FUEL\_DENS 1773.0

\*

\*000002 CLAD\_CREEP

000002 CLAD\_SWEL

000002 CLAD\_PLAS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* RESTART CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno r1 s1

000005 0 1

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* INITIAL TEMPERATURE CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno tem0

000006 651.

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* INITIAL AXIAL DIVISION

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno dz0 nz nfr

000003 0.025 8 1

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL GEOMETRY CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno fmat fden pucont rfi rfo ruff stoch nf nfr

100001 mox 10410. 0.45 1.0E-3 2.71E-3 3.0E-6 2.0 22 1

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* GAP CARDS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno gmat dgap pin vpl nfr

\*100002 he 1.15E-4 1.0E+5 1.4518E-6 1

100002 he 1.15E-4 1.0E+5 1.E-4 1

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL ROD CLADDING CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno cmat rco cden rufc nc nfr

100003 aim1 3.275E-3 7900. 1.0E-6 5 1

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* POWER CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno time qv

300000 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00

300000 3.60E+03 1.04E+09 1.11E+09 1.19E+09 1.24E+09 1.35E+09 1.40E+09 1.46E+09 1.51E+09

300000 7.33E+06 1.04E+09 1.11E+09 1.19E+09 1.24E+09 1.35E+09 1.40E+09 1.46E+09 1.51E+09

300000 7.34E+06 1.09E+09 1.19E+09 1.26E+09 1.32E+09 1.42E+09 1.49E+09 1.54E+09 1.57E+09

300000 1.66E+07 1.09E+09 1.19E+09 1.26E+09 1.32E+09 1.42E+09 1.49E+09 1.54E+09 1.57E+09

300000 1.67E+07 1.07E+09 1.17E+09 1.23E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.52E+09

300000 1.96E+07 1.07E+09 1.17E+09 1.23E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.52E+09

300000 1.97E+07 1.08E+09 1.17E+09 1.24E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.58E+09

300000 2.11E+07 1.08E+09 1.17E+09 1.24E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.58E+09

300000 2.12E+07 1.06E+09 1.12E+09 1.20E+09 1.30E+09 1.34E+09 1.41E+09 1.47E+09 1.52E+09

300000 2.57E+07 1.06E+09 1.12E+09 1.20E+09 1.30E+09 1.34E+09 1.41E+09 1.47E+09 1.52E+09

300000 2.58E+07 9.21E+08 9.60E+08 1.04E+09 1.11E+09 1.17E+09 1.22E+09 1.28E+09 1.32E+09

300000 3.75E+07 9.21E+08 9.60E+08 1.04E+09 1.11E+09 1.17E+09 1.22E+09 1.28E+09 1.32E+09

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL STOICHIOMETRY VS BURNUP

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno bup stoich

400005 0.0 2.0

400005 100. 2.0

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* COOLANT CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno ctype dhyd xarea press flowr tcoolin

500000 na 3.65E-03 3.3E-05 2.0E+05 1.07E-01 6.51E+02

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* BASE IRRADIATION TIME CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno tstart tend dtout

600000 0.0 3.75E+07 86400.0

\*crdno tout

600001 3.60E+03

600001 7.33E+06

600001 7.33E+06

600001 1.66E+07

600001 1.66E+07

600001 1.96E+07

600001 1.96E+07

600001 2.11E+07

600001 2.11E+07

600001 2.57E+07

600001 2.58E+07

600001 3.75E+07

$

**Time integration card (crdno=000000)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* TIME INTEGRATION CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno meth rtol atol hmax

000000 GEAR0 1.0E-5 1.E-5 7200.

1. **meth**: time integration method indicator:

GEAR0 – backward differentiation formula with automatically  
generated Jacobi matrix;

1. **rtol**: relative tolerance parameter;
2. **atol**: absolute tolerance parameter.
3. **hmax** - maximum allowable time step

**Transient card (crdno=000001)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* TRANSIENT CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno itran nout ntrac

000001 0 1 0

1. **itran**: transient indicator:

0 – steady-state calculation;

1 – transient calculation;

1. **nout**: output frequency (FRED output is written each **nout** time steps).
2. **ntrac**: frequency of FRED call from TRAC

**Options card (crdno=000002)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* OPTION CARDS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

000002 OUTPUT\_AXIAL\_LAYER 4

000002 OUTPUT\_FUEL\_ROD 1

\*

000002 FGR

000002 FUEL\_CREEP

000002 FUEL\_SWEL

\*000002 FUEL\_PLAS

000002 FUEL\_DENS 1773.0

\*

\*000002 CLAD\_CREEP

000002 CLAD\_SWEL

000002 CLAD\_PLAS

1. **OUTPUT\_AXIAL\_LAYER**: output reference axial layer
2. **OUTPUT\_FUEL\_ROD**: output reference fuel rod
3. **FGR**: flag of fission gas release calculation
4. **FUEL\_CREEP**: flag of fuel creep calculation
5. **FUEL\_SWEL**: flag of fuel swelling calculation
6. **FUEL\_PLAS**: flag of fuel plasticity calculation
7. **FUEL\_DENS**: fuel sintering temperature (K)
8. **CLAD\_CREEP**: flag of clad creep calculation
9. **CLAD\_SWEL**: flag of clad swelling calculation
10. **CLAD\_PLAS**: flag of clad plasticity calculation

**Restart card (crdno=000005)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* RESTART CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno r1 s1

000005 0 1

* 1. **r1**: option for reading fuel rod temperatures from RSTFRD file:

0: do not read temperatures from restart file;

1: read temperatures from restart file;

1. **s1**: option for writing fuel rod temperatures to RSTFRD file:

0: do not save temperatures in restart file;

1: save temperatures in restart file.

**Initial temperature card (crdno=000006)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* INITIAL TEMPERATURE CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno tem0

000006 651.

1. **tem0**: initial temperature (K).

One and the same temperature is written in all FRED structures at the beginning of a new calculation.

**Fuel rod axial division card (crdno=000003)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* INITIAL AXIAL DIVISION

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno dz0 nz nfr

000003 0.025 8 1

1. **dz0**: axial slice height (m)
2. **nz**: number of slices
3. **nfr**: number of fuel rods with such parameters.

**Fuel pellet card (crdno=100001)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL GEOMETRY CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno fmat fden pucont rfi rfo ruff stoch nf nfr

100001 mox 10410. 0.45 1.0E-3 2.71E-3 3.0E-6 2.0 22 1

1. **fmat**: fuel type:  
   UO2: uranium dioxide;

MOX: mixed uranium-plutonium dioxide;

BN: boron nitride.

1. **fden**: fuel density (kg/m3);
2. **pucont**: plutonium content (rel.units);
3. **rfi**: radius of fuel pellet inner hole (m);
4. **rfo**: outer radius of fuel pellet (m);
5. **ruff**: roughness of outer surface of fuel pellet (m);
6. **nf**: number of radial nodes in fuel pellet;
7. **nfr**: number of fuel rods with such parameters.

**Fuel-clad gap card (crdno=100002)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* GAP CARDS

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno gmat dgap pin vpl nfr

\*100002 he 1.15E-4 1.0E+5 1.4518E-6 1

100002 he 1.15E-4 1.0E+5 1.E-4 1

1. **gmat**: material in fuel-clad gap:  
   HE: helium;  
   PB: lead;
2. **dgap**: initial fuel-clad gap width (m);
3. **pin**: initial gas pressure inside fuel rod (Pa);
4. **vpl**: initial gas plenum volume (m3);
5. **nfr**: number of fuel rods with such parameters.

All data are for cold conditions.

**Fuel rod cladding card (crdno=100003)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL ROD CLADDING CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno cmat rco cden rufc nc nfr

100003 aim1 3.275E-3 7900. 1.0E-6 5 1

1. **cmat**: cladding type:  
   SS823: stainless steel EP-823 (12%Cr-Si);

SS316: stainless steel SS316;

AIM1: Austenitic Improved Material 1;

T91: 9Cr–1MoVNb type steel.

1. **rco**: cladding outer radius (m);
2. **cden**: cladding density (kg/m3);
3. **rufc**: roughness of cladding inner surface (m);
4. **nc**: number of radial nodes in cladding;
5. **nfr**: number of fuel rods with such parameters.

**Fuel power card (crdno=300000)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* POWER CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno time qv

300000 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00

300000 3.60E+03 1.04E+09 1.11E+09 1.19E+09 1.24E+09 1.35E+09 1.40E+09 1.46E+09 1.51E+09

300000 7.33E+06 1.04E+09 1.11E+09 1.19E+09 1.24E+09 1.35E+09 1.40E+09 1.46E+09 1.51E+09

300000 7.34E+06 1.09E+09 1.19E+09 1.26E+09 1.32E+09 1.42E+09 1.49E+09 1.54E+09 1.57E+09

300000 1.66E+07 1.09E+09 1.19E+09 1.26E+09 1.32E+09 1.42E+09 1.49E+09 1.54E+09 1.57E+09

300000 1.67E+07 1.07E+09 1.17E+09 1.23E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.52E+09

300000 1.96E+07 1.07E+09 1.17E+09 1.23E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.52E+09

300000 1.97E+07 1.08E+09 1.17E+09 1.24E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.58E+09

300000 2.11E+07 1.08E+09 1.17E+09 1.24E+09 1.31E+09 1.39E+09 1.43E+09 1.50E+09 1.58E+09

300000 2.12E+07 1.06E+09 1.12E+09 1.20E+09 1.30E+09 1.34E+09 1.41E+09 1.47E+09 1.52E+09

300000 2.57E+07 1.06E+09 1.12E+09 1.20E+09 1.30E+09 1.34E+09 1.41E+09 1.47E+09 1.52E+09

300000 2.58E+07 9.21E+08 9.60E+08 1.04E+09 1.11E+09 1.17E+09 1.22E+09 1.28E+09 1.32E+09

300000 3.75E+07 9.21E+08 9.60E+08 1.04E+09 1.11E+09 1.17E+09 1.22E+09 1.28E+09 1.32E+09

This card defines the fuel rod power density in table of fuel rod power density vs time.

1. **time**: time array corresponding to qv (s);
2. **qv**: array of fuel rod power density vs time (W/m3)

**Fuel stoichiometry card (crdno=400005)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* FUEL STOICHIOMETRY VS BURNUP

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno bup stoich

400005 0.0 2.0

400005 100. 2.0

This card is used, as a rule, for simulation of fuel stoichiometry under steady-state.

1. **bup**: fuel burnup (at%);
2. **stoich**: fuel stoichiometry.

**Coolant card (crdno=300000)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* COOLANT CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno ctype dhyd xarea press flowr tcoolin

500000 na 3.65E-03 3.3E-05 2.0E+05 1.07E-01 6.51E+02

1. **ctype**: coolant type:

Na: sodium coolant;

He: helium gas;

Pb: lead coolant;

PbBi: lead-bismuth coolant.

1. **dhyd**: hydraulic diameter of the channel (m);
2. **xarea**: cross-sectional area of the channel (m2);
3. **press**: coolant pressure (Pa);
4. **flowr**: flowrate (kg/s);
5. **tcoolin**: inlet coolant temperature (K).

**Base-irradiation time card (crdno=600000)**

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\* BASE IRRADIATION TIME CARD

\*---- ----1---- ----2---- ----3---- ----4---- ----5---- ----6---- ----7---- ----8---- ----9--

\*crdno tstart tend dtout

600000 0.0 3.75E+07 86400.0

1. **tstart**: start time (s);
2. **tend**: end time (s);
3. **dtout**: output time step (s).

**Base-irradiation output time card (crdno=600001)**

\*crdno tout

600001 3.60E+03

600001 7.33E+06

600001 7.33E+06

600001 1.66E+07

600001 1.66E+07

600001 1.96E+07

600001 1.96E+07

600001 2.11E+07

600001 2.11E+07

600001 2.57E+07

600001 2.58E+07

600001 3.75E+07

$

1. **tout**: output time (s).
2. **$**: symbol of the end of input deck.

## Running FRED

Create a working folder to run calculation cases (for example, input files in path */user/FRED/01.FRED.RUN*):

mkdir /user/FRED/01.FRED.RUN

cd /user/FRED/01.FRED.RUN

### Running method 1

In the working folder, create a *run* batch file with following contents:

/user/FRED/00.FRED.SRC/fred.x

With both the *run* batch file and input deck *fred* in the working folder, executing command:

./run

### Running method 2

For users using supercomputers or computer clusters, it is recommended to utilize the Slurm Workload Manager to mange jobs.

In the working folder, create a *Slurm.sh* batch file. Below are listed the common settings:

#!/bin/bash

#SBATCH --partition=hourly # Using 'hourly' will grant higher priority

#SBATCH --ntasks-per-core=1 # Force no Hyper-Threading, will run 1 task per core

#SBATCH --time=00:59:59 # Define max time job will run

#SBATCH --output=fred.out # Define your output file

#SBATCH --error=fred.err # Define your error file

/user/FRED/00.FRED.SRC/fred.x

With both the *Slurm.sh* batch file and input deck *fred* in the working folder, submit the job:

sbatch Slurm.sh

All running jobs of user can be viewd by:

squeue –u user\_name

## Results and Post-processing

The main calculational results are written with a specified frequency to the output data file *fred.dat*. The values of key parameters over time are recorded in this file. a brief description of the output parameters are given in Table 1.

Table 1 Description of parameters in output file

|  |  |  |
| --- | --- | --- |
| Name | Units | Description |
| temfi | ℃ | Fuel temperature on inner surface |
| temfo | ℃ | Fuel temperature on outer surface |
| temci | ℃ | Clad temperature on inner surface |
| temco | ℃ | Clad temperature on outer surface |
| tfave | ℃ | Radially-average fuel temperature |
| tcave | ℃ | Radially-average clad temperature |
| hgap | W/K-m2 | Heat conductance of the fuel-clad gap |
| rfi | mm | Fuel pellet inner radius |
| rfo | mm | Fuel pellet outer radius |
| rci | mm | Clad inner radius |
| rco | mm | Clad outer radius |
| gap | μm | Radial fuel-clad gap width |
| gapth | μm | "thermal" gap width |
| gpres | MPa | Plenum gas pressure |
| pfc | MPa | Pellet-to-cladding contact pressure |
| htc | W/K-m2 | Clad-to-coolant heat transfer coefficient |
| fgrpp | % | Fission gas release fraction |
| efs | % | Fuel linear swelling strain |
| gap\_state | - | flag of gap state (closed or open) |

If the restart writing option (in the Restart card part) is active in the input deck, RSTFRD files will be generated. The data in RSTFRD files can be extracted by running python script *data\_to\_csv.py*:

Python data\_to\_csv.py

It is noted that the “timestep” and “r\_central\_line” should be modified according to the setting in input deck.

# Brief description of FRED modeling

## Fuel rod nodalization scheme

A three-dimensional cylindrical geometry is used in the fuel rod nodalization scheme. The calculational nodes are located only on the active part of the fuel rod.

The scheme of division of the calculational region of the control volumes in the radial, tangential and axial directions as well as the location of the calculational nodes for temperature is shown in **Figure 1** for the calculational region with a central hole and in **Figure 2** for the calculational region without a central hole. A uniform distribution over a circumference is assumed: .



**Figure 1** Distribution of calculational nodes for temperature

in the calculational region with central hole



**Figure 2** Distribution of calculational nodes for temperature  
in the calculational region without central hole

The feature of the scheme is a coincidence of the boundaries between materials with the temperature nodes located on the material boundaries.

## Governing equations

### Heat transfer

The differential equation for heat transfer is solved in the calculational area in cylindrical geometry with account for radial, tangential and axial heat fluxes in the solid material:



where: *ρ* – density (kg/m3);

*cp* – specific heat (J/kg-K);

*λ* – thermal conductivity (W/m-K);

*qv* – power density (W/m3);

*r,θ,z* – coordinates in cylindrical geometry (m);

*τ* – time (s).

The power density distribution is calculated in the TRAC/AAA point kinetics model or in the PARCS spatial kinetics model and sent to the FRED model at each time step.

The following ordinary differential equations (ODE) are derived by discretization of Eq. for control volume i:



where: – heat flux between volumes j and i (W/m2).

The sum in Eq.is taken over all “neighbouring” volumes, while the heat flux between volumes i and j is determined as:



where:  – thermal conductivity of the material between centres of volumes j and i (W/m-K);

 – distance between the centres of volumes j and i (m).

When heat transfer is calculated through the fuel-clad gap, the heat flux is determined as:



where:  – gap conductance between surface of cladding j fuel i (W/m2-K).

When heat transfer is calculated from clad to coolant, the heat flux is determined as:



where:  –heat transfer coefficient between coolant j and cladding i (W/m2-K).

### Stress-strain condition

Tangential (hoop), radial and axial components of the total fuel and clad deformations are calculated taking into account elastic strain, thermal expansion, swelling and creep under the followings assumptions:

* these components are additive
* shear stresses and shear strains are assumed zero
* the total axial deformation is constant over the fuel radius (thickness of each axial slice remains constant with radius): εz=const;
* the total axial deformation is constant over the cladding radius: εz =const;
* there is no axial slip between the fuel and cladding in the pellet cladding mechanical interaction (PCMI) regime.

*Deformation components* are by definition correlated with cladding displacements as follows:







where:  –the tangential, radial and axial components of the total cladding deformation (m/m);

u and w – the radial and axial displacement, respectively (m);

r and z – the radial and axial coordinates, respectively (m).

*Deformation compatibility equation* in radial direction:



*Stress equilibrium equation* in radial direction:



*Hook’s equation for each axial slice*:







where  –the tangential, radial and axial components of thermal-viscous-plastic deformation (m/m);

 – tangential, radial and axial components of cladding stress (Pa);

Е – Young modulus of the cladding material (Pa);

ν – Poisson’s ratio of the cladding material.

*Effective stress* is calculated by the Hill equation:



*The boundary conditions* for the cladding stress-strain model in the open fuel-clad gap regime are defined by the following equations:





and the integral equation for the balance of axial stresses:



where Pi – is the gas pressure inside fuel rod;

Pо – is the coolant pressure;

ri and rо – are the inner and outer cladding radii.

The condition of switching to the closed gap regime is equality for the given axial slice of the outer radius of the fuel pellet and the inner radius of the cladding. In this regime, according to the accepted assumptions about absolutely solid fuel and absence of slipping between fuel and cladding, the boundary conditions are determined by equality of linear cladding and fuel pellet deformation rates for axial and tangential components:





where: εf – is the fuel outer surface deformation;

symbol Δ denotes increment of the value in the time integration step.

*Contact pressure* under conditions of the closed gap is assumed equal to the radial stress component on the inner clad surface taken with an opposite sign. The criterion of the gap re-opening is decrease of the contact pressure below the gas pressure inside the fuel rod.

The radial distribution of the components of the *thermal-viscous-plastic deformation*, included in the right-hand sides of Eqs- are determined for each axial slice under the assumption that all elements are additive:



where ;

 – clad thermal expansion;

 – clad creep;

 – clad plastic deformation.

Creep components are determined by time integration of equations written according to the Prandtl-Reuss flow rules with the use of empirical correlations for the effective creep rate:



where ;

σ(r,z) – effective stress (Pa);

R – universal gas constant (J/mol-K);

T(r,z) – clad temperature (K);

A, Q and η – empirical constants.

To calculate clad plastic deformation components a mono-axial plastic deformation curve based on experimental data in MATPRO report [10] is integrated over the time with respect to the effective deformation. (It is accepted that the data given in [10] is for LWRs and this will be modified in the future for other materials):

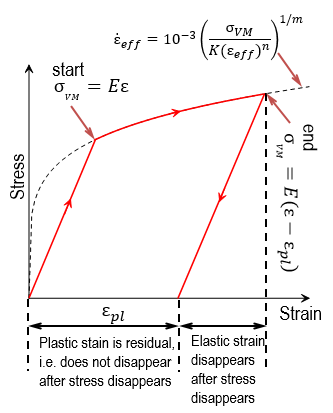


where ε – is the effective deformation;

К – is the strength coefficient;

n – is the strain hardening exponent;

m – is the strain rate sensitivity exponent.



**Figure 3** Clad uniaxial deformation curve

The coefficients used in Eq. are empirical functions of temperature and neutron fluence. The clad plastic deformation in a node begins when the following condition is met in this node:



where σ – is the effective stress from Eq.;

E – Young modulus;

ε – the effective deformation calculated from Eq..

After start of plasticity, the effective plastic deformation is determined at each time step as



The components of plastic deformation are determined by time integration of equations written according to the Prandtl-Reuss flow rules:



where ;

– is the effective deformation rate, calculated by Eq..

The plastic deformation stops, when the following condition is met:



where  – is the effective plastic deformation, calculated at previous time step.

The cladding nodalization scheme for n control volumes distributed between the inner and outer radii and the disposition of the calculational nodes for the stress and deformation components are shown in **Figure 4**. The feature of this scheme is that the first and last nodes are located on the inner and outer clad surfaces, respectively.



**Figure 4** Calculational nodes for stress and deformation components in cladding

The discretization of Eqs - and - for the chosen nodalization scheme makes it possible to write for each axial slice a set of equations, as follows:

















The set of linear (5n-2) algebraic equations - is solved with standard methods of LU-decomposition and back substitution [2] with respect to components of the total deformation and stresses. The resulting vector has the form:

.

The set of ordinary differential equations (ODE) includes equations for fuel and cladding temperatures, for creep components, for the effective deformation and for plastic deformation components. Such a system of ODEs is solved for each fuel rod and/or other structural elements with the use of the standard subroutine LSODES [3].

The set of linear equations - is solved at each time step in an iteration cycle including the recalculation of the gas pressure inside the fuel rod, which is necessary due to changes in the fuel rod geometry being accounted for as follows:





where  – the current and initial radii of calculational node i, respectively;

 – the current and initial height of calculational axial slice j, respectively.

# Specific material and behaviour models

## Fuel material models

### Fuel thermal conductivity [Flamb]

#### UO2

The thermal conductivity of UO2 available in FRED refers to the research of Harding and Martin[4]. The equation is given as:













where:  – thermal conductivity of the UO2 (W/m-K);

 – thermal conductivity of the unirradiated UO2 (W/m-K);

 – burnup (MWd/kgU);

 – temperature (K);

 – factor of dissolved fission products. When =0, =1;

 – factor of precipitated fission products. When =0, =1;

 – factor of fuel porosity effect;

 – factor of radiation effect;

 – fuel porosity.

#### MOX

According to the research of Philipponneau [5], the thermal conductivity of MOX fuel is proposed as:



where:  – thermal conductivity of the MOX fuel (W/m-K);

 – parameter about stoichometry;

 – temperature (K);

 – fuel porosity.

The parameter about stoichometry  is determined as:



where: – fuel stoichiometry;

 – burnup (MWd/kgU);

The fuel porosity  is determined as:





where: – fuel density (kg/m3);

– theoretical fuel density (kg/ m3);

 – plutonium fraction.

#### UC

The thermal conductivity of UC is obtained from the research of Lewis and Kerrisk [6]:



where:  – thermal conductivity of UC (W/m-K);

 – temperature (K);

 – temperature (℃), i.e. -273.15K.

The thermal conductivity of PuC:



where:  – thermal conductivity of PuC (W/m-K);

 – temperature (℃).

In FRED code, it considers that the thermal conductivity of PuC is not greater than that of UC, otherwise the calculation of PuC thermal conductivity refers to Eq..

Then the mixed (U-Pu)C thermal conductivity is given as:



where:  – thermal conductivity of (U-Pu)C (W/m-K);

 – plutonium fraction.

#### UN

The thermal conductivity of UN is determined as:



where:  – thermal conductivity (W/m-K);

 – plutonium fraction;

 – temperature (K);

 – fuel porosity.

The fuel porosity  is determined as:





where: – fuel density (kg/m3);

– theoretical fuel density (kg/ m3);

#### BN

The thermal conductivity of BN refers to program TRACE V5 [7][8]:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

### Fuel specific heat [Fcp]

#### UO2 and MOX

The specific heat of UO2 or MOX is given as:



where:  – fuel specific heat (J/kg-K);

 – UO2 specific heat (J/kg-K);

 – PuO2 specific heat (J/kg-K);

 – plutonium fraction.

The  and  can be obtained by interpolation from the experimental data of Popov. et.al[9]:

Table 2 data of  and 

|  |  |  |
| --- | --- | --- |
| T(K) | (J/kg-K) | (J/kg-K) |
| 300 | 235.51 | 203.71 |
| 400 | 265.79 | 225.79 |
| 500 | 282.14 | 235.77 |
| 600 | 292.21 | 241.33 |
| 700 | 299.11 | 244.92 |
| 800 | 304.24 | 247.47 |
| 900 | 308.32 | 249.44 |
| 1000 | 311.74 | 251.04 |
| 1100 | 314.76 | 252.43 |
| 1200 | 317.59 | 253.70 |
| 1300 | 320.44 | 254.96 |
| 1400 | 323.60 | 256.32 |
| 1500 | 327.41 | 257.93 |
| 1600 | 332.31 | 259.93 |
| 1700 | 338.77 | 262.47 |
| 1800 | 347.30 | 265.67 |
| 1900 | 358.40 | 269.57 |
| 2000 | 372.54 | 274.17 |
| 2100 | 390.12 | 279.35 |
| 2200 | 411.46 | 284.96 |
| 2300 | 436.78 | 290.80 |
| 2400 | 466.21 | 296.70 |
| 2500 | 499.80 | 302.47 |
| 2600 | 537.50 | 308.00 |
| 2700 | 579.17 | 313.21 |
| 2800 | 624.63 | 318.08 |
| 2900 | 673.63 | 322.59 |
| 3000 | 725.88 | 326.76 |
| 3100 | 781.08 | 330.64 |

Account for the melting of fuel, the specific heat of UO2 and MOX is described by the equation:



where:  – temperature (K);

 – melting point (K).

The melting point  is given as:



where:  – plutonium fraction.

#### UC

The specific heat of UC can be obtained by interpolation from the following data:

Table 3 data of UC specific heat

|  |  |
| --- | --- |
| Temperature(K) | specific heat of UC(J/kg-K) |
| 293 | 207 |
| 500 | 216 |
| 700 | 225 |
| 900 | 234 |
| 1100 | 243 |
| 1300 | 253 |
| 1500 | 264 |
| 1700 | 275 |
| 1900 | 288 |
| 2100 | 301 |
| 2300 | 316 |
| 2500 | 332 |
| 2700 | 350 |
| 2775 | 357 |
| 2780 | 54443 |
| 2785 | 357 |
| 5000 | 357 |

#### UN

The specific heat of UN:





where:  – fuel specific heat (J/kg-K);

 – temperature (K), 293 K≤≤4000 K.

#### BN

The specific heat of BN refers to program TRACE V5 [7][8]:





where:  – fuel specific heat (J/kg-K);

 – temperature (K).

### Fuel Young’s modulus [Felmod]

#### UO2 and MOX

The models of Young’s modulus for UO2 or MOX is taken from MATPRO report [10]:



where:  – fuel Young’s modulus (Pa);

 – fuel temperature (K);

 – plutonium fraction;

 – fuel porosity.

The fuel porosity  is determined as:gand





where: – fuel density (kg/m3);

– theoretical fuel density (kg/ m3).

#### BN

The Young’s modulus of BN is considered as Pa.

### Fuel Poisson ratio [Fpoir]

#### UO2

The value of Poisson ratio for UO2 is



#### MOX

The Poisson ratio of MOX fuel:



#### BN

The Poisson ratio of BN:



### Fuel fracture strength [Fsigf]

In FRED, the MATPRO model is used to calculate the fracture strength of UO2 and MOX fuel [10]:



where:  – fuel fracture strength (Pa);

 – universal gas constant = 8.314 J/K-mol;

 – fuel temperature (K);

 – fuel porosity.

The fuel porosity  is determined as:





where: – fuel density (kg/m3);

– theoretical fuel density (kg/ m3);

 – plutonium fraction.

### Fuel thermal expansion [Ftexp]

Thermal expansion is the tendency of a matter to change in volume in response to a change in temperature.

#### UO2 and MOX

The equations for thermal expansion of UO2 or MOX are taken from MATPRO report [10]:



where:  – fuel linear strain caused by thermal expansion;

 – UO2 linear strain caused by thermal expansion;

 – PuO2 linear strain caused by thermal expansion;

 – plutonium fraction.

The linear strain caused by thermal expansion of UO2 or PuO2 is calculated by:





where:  – fuel temperature (K).

#### UC

Based on K.Mikityuk’s research in the GFR report GCFR-DEl-011, the thermal expansion strain of UC is given as:



where:  – fuel linear strain caused by thermal expansion;

– fuel temperature (℃).

#### UN

The thermal expansion strain of UN is described as:



where:  – fuel linear strain caused by thermal expansion;

 – fuel temperature (K).

#### BN

The thermal expansion strain of BN is described as:



where:  – fuel linear strain caused by thermal expansion;

 – fuel temperature (K).

### Fuel creep [Fceep]

Creep is slow movement of material under the influence of stresses (that are still below the yield strength) induced by thermal expansion, swelling and pressure difference: inner gas/coolant. Creep behaviour has a tendency to relax these stress.

The creep strain of MOX fuel is taken account in FRED code. Several models are implemented.

#### LIFE-GCFR model

In the LIFE-GCFR model, the fuel creep consists of four parts [11]:

1) Athermal fission-induced creep at low temperature (T< 300 ℃)



where:  – athermal fission-induced creep rate (1/h);

 – constant, 3.72×10-23;

 – fission rate (fission/cm3-s);

 – effective stress (Psi), 1 Pa = 0.000145 Psi.

2) radiation-enhanced creep (300 ℃ <T< 1200 ℃)



where:  – radiation-enhanced creep rate (1/h);

 – constant = 1.96×10-19;

 – active energy = 13.7×103 cal/mol;

 – universal gas constant = 1.98722 cal/K-mol;

 – fuel temperature (K).

3) viscous thermal creep at high temperature (T> 0.5Tm, Tm is the melting point)



where:  – viscous thermal creep rate (1/h);

 – constant = 2.23×107;

 – constant = 20;

 – active energy = 92.5×103 cal/mol;

4) thermal creep at high temperature and high stress



where:  – viscous thermal creep rate (1/h);

 – constant = 1.0×10-3;

 – active energy = 136.8×103 cal/mol;

In computing the total creep rate, the effect of fuel density must be taken into account:



where:  – total creep rate (1/h);

– fuel density (%TD);

#### SAS4A model

The creep rate in this model is described as:



where:  – creep rate (1/h);

 – effective stress (MPa);

 – universal gas constant = 1.98722 cal/K-mol;

 – fuel temperature (K).

#### URANUS model

According to the study of Lassmann and Moreno [12], the fuel creep rate given as:









where:  – total creep rate (1/h);

 – fission rate (fission/cm3-s);

 – effective stress (Psi);

 – constant = 20;

 – universal gas constant = 1.98722 cal/K-mol;

 – fuel temperature (K).

In the current version of FRED, the SAS4A model is used.

### Fuel swelling [Fswel]

The swelling behaviour can be included into the simulation of UO2 and MOX fuel. In FRED, the swelling strain can be set in the input file as a table of fuel swelling (%) vs. fuel burnup (MWd/kgU) or calculated by built-in physical models.

#### MATPRO model

In MATPRO model [10], two components to the fuel swelling due to irradiation are identified:

1. a swelling connected to the buildup of solid fission products and limited to approximately 0.5 to 1.0% ΔV/V per 10 MWd/kgU (~1 at%) and
2. a swelling connected to gas pressure in fuel pores (depends on the fission gas release).

The correlation to calculate swelling caused by solid fission products is given as:



where:  – volumetric swelling strain due to solid fission products;

 – burnup during a time step (fissions/m3).

At temperatures below 2800K, fuel swelling due to the gaseous fission products is considered:



where:  – volumetric swelling strain due to gaseous fission products;

 – burnup during a time step (fissions/m3);

 – total burnup (fissions/m3).

#### Simple model

Actually, in current version of FRED, a simple model is used to calculating the fuel swelling strain:

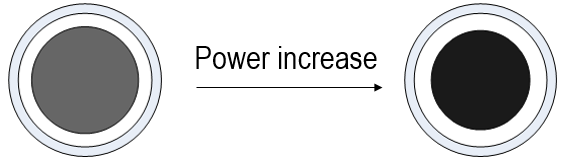


where:  – volumetric swelling strain;

 – burnup during a time step (FIMA%).

### Fuel densification [Fdens]

Ceramic fuel densification is an increase of effective fuel density (up to few %) at early stage of irradiation and therefore reduction of the fuel pellet radius.



**Figure 5** Fuel densification

Fuel densification is caused by disappearance of small pores and defects under conditions of temperature elevation. It contributes to fuel temperature increase at beginning of irradiation.

In FRED, the following equation is used to calculate the maximum fuel densification strain:



where:  – maximum fuel densification strain;

 – sintering temperature (K);

 – fuel porosity (%).

The fuel porosity  is determined as:





where: – fuel density (kg/m3);

– theoretical fuel density (kg/ m3);

 – plutonium fraction.

Then the densification as a function of burnup is calculated using



where:  –fuel densification strain;

 – burnup (MWd/kgHM);

 – a constant determined by iteration to fit the condition: when B=0, ∆L/L = 0.

### Fission gas release [FGR]

In FRED, the fission gas release fraction can be set in the input file as a table of release fraction vs. fuel temperature or calculated by built-in physical models.

#### UO2 and MOX

According to the study of Waltar and Reynolds [13], the fraction of fission gas release is



where:  – fraction of fission gas release;

 – release fraction for the restructured region;

 – release fraction for the unrestructured region;

, – fractional fuel areas associated with the restructured or unrestructured region.

The release fraction for the restructured regions and the unrestructured region:







where:  – burnup (MWd/kgHM);

 – local linear power (kW/m).

 is set equal to zero when it yields a negative number.

In current version of FRED, all fuel region is assumed to be unrestructured.

#### UN

For the UN fuel, the fission gas release fraction is given as:



where:  – fraction of fission gas release;

 – burnup (FIMA%).

#### UC

As recommended in the research of Preusser [14], the fission gas begins when the burnup exceeds the limited value:



where:  –the percent of burnup at which fission gas release begins (FIMA%);

 – temperature (℃).

Then the fission gas release in percent is given as:



where:  –fission gas release in percent (%).

It was taken that with very high burnups the fission gas release rate approaches a constant value, so the equation is modified as:



where:  – burnup (FIMA%).

### Burnup [Baseir]

The fuel rod burnup is calculate as:



where:  – burnup(MWd/kgU);

 – initial burnup (MWd/kgU);

 – power density (W/m3);

 – fuel density (kg/m3);

 – time increment (s).

## Cladding material models

### Cladding thermal conductivity [Clamb]

#### ZrN

The equation of the thermal conductivity for ZrN:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### Zry

The thermal conductivity for Zry is given as:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### SS823

The thermal conductivity for SS823 alloy is determined as:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### AIM1

The thermal conductivity for AIM1 cladding material is



where:  – thermal conductivity (W/m-K);

 – temperature (℃).

#### SS316

The thermal conductivity for SS316 alloy is determined as:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### T91

The thermal conductivity for T91 cladding material is



where:  – thermal conductivity (W/m-K);

 – temperature (℃).

### Cladding Young’s modulus [Celmod]

#### SS823

The models of Young’s modulus for SS823 alloy is determined as:



where:  – Young’s modulus (Pa);

 – temperature (K).

#### AIM1

The Young’s modulus for AIM1 cladding material is



where:  – Young’s modulus (Pa);

 – temperature (℃).

#### T91

The Young’s modulus for T91 cladding material is given as:



where:  – Young’s modulus (Pa);

 – temperature (℃).

#### SS316

The Young’s modulus for SS316 alloy is determined as:



where:  – Young’s modulus (Pa);

 – temperature (K).

### Cladding Poisson ratio [Cpoir]

#### AIM1

The value of Poisson ratio for AIM1 alloy is



#### SS823

The value of Poisson ratio for SS823 alloy is given as



#### SS316

The value of Poisson ratio for T91 alloy is given as



#### T91

The value of Poisson ratio for T91 alloy is given as



### Cladding burst stress [Csigb]

#### SS823

The burst stress of SS823 alloy is from the linear interpolation for the data listed in the following table:

Table 4 Burst stress database for SS823

|  |  |
| --- | --- |
| Temperature(K) | Burst stress (MPa) |
| 293 | 975 |
| 573 | 764 |
| 623 | 745 |
| 673 | 686 |
| 723 | 642 |
| 773 | 558.5 |
| 873 | 367.5 |
| 923 | 274.5 |
| 973 | 172 |
| 1053 | 72 |
| 1173 | 47 |
| 1273 | 30 |
| 1373 | 23 |
| 1473 | 13 |

#### AIM1 and T91

The burst stress of AIM1 and T91 alloy is



where:  – burst stress (Pa);

 – temperature (K).

#### SS316

The burst stress of SS316 alloy is given as



where:  – burst stress (MPa);

 – temperature (℃).

### Cladding yield stress [Csigy]

#### SS823

The yield stress of SS823 alloy is from the linear interpolation for the data listed in the following table:

Table 5 Yield stress database for SS823

|  |  |
| --- | --- |
| Temperature(K) | Burst stress (MPa) |
| 293 | 960.5 |
| 573 | 749.5 |
| 623 | 720.5 |
| 673 | 676 |
| 723 | 632 |
| 773 | 553.5 |
| 873 | 362.5 |
| 923 | 264.5 |
| 973 | 162 |
| 1053 | 68 |
| 1173 | 42 |
| 1273 | 27 |
| 1373 | 21 |
| 1473 | 12 |

#### AIM1

The value of yield stress for AIM1 alloy is



where:  – yield stress (Pa);

 – temperature (℃).

#### T91

The yield stress of T91 alloy is



where:  – yield stress (Pa);

 – temperature (K).

#### SS316

The yield stress of SS316 alloy is given as



where:  – yield stress (MPa);

 – temperature (℃).

### Cladding thermal expansion [Ctexp]

#### AIM1

The equations for thermal expansion of AIM1 alloy is given as:



where:  – linear strain caused by thermal expansion;

 – temperature (℃).

#### SS823, T91 and SS316

For SS823, T91 or SS316 alloy, the equation of thermal expansion is



where:  – linear strain caused by thermal expansion;

 – temperature (K).

### Cladding creep [Cceep]

#### AIM1

The creep model of AIM1 alloy in FRED is obtained from the research of Choudhary and Samuel [15], given as:



where:  – creep rate (1/h);

 – effective stress (MPa);

 – temperature (K).

The creep rate is considered not exceed 1.0×10-4 h-1.

#### Other claddings

For the creep rate of other cladding material calculated by FRED, it shares the equation:



where:  – creep rate (1/h);

 – effective stress (MPa);

 – temperature (K).

The creep rate is considered not exceed 1.0×10-4 h-1.

The creep results in relaxation of stresses however too large creep can cause clad failure.

### Cladding swelling [Cswel]

#### SS823

The swelling strain of the SS823 alloy:



where:  – volumetric swelling strain;

 – temperature (℃).

 – displacement per atom, 1=1.4087*B*, where *B* is the burnup in MWd/kgU.

#### T91

Roche correlation from Michael Schikorr (?) is used to calculate the swelling strain of T91:



where:  – volumetric swelling strain;

 – displacement per atom.

In this model, 1=1.4087×1.35B, *B* is the burnup in MWd/kgU.

As for the parameter,  and :







#### AIM1

The swelling model of AIM1 is taken from Luzzi et al (?), the swelling strain is given as:



where:  – volumetric swelling strain;

 – temperature (℃);

 – fast neutron fluence (1022 n/cm2). The conversion between fluence and dpa

is 2×1021 (n/cm2)/dpa.

Based on CAPRIX test data, in this model, 1=0.4156*B*, *B* is the burnup in MWd/kgU.

### Cladding ultimate elongation [Cuelon]

As shown in Figure 6, the plastic strain at maximum load is typically referred to as the ultimate elongation (εu), which is calculated in FRED.



**Figure 6** Stress vs. strain curve

#### SS823

The ultimate elongation of SS823 alloy is from the linear interpolation for the data listed in the following table:

Table 6 Yield stress database for SS823

|  |  |
| --- | --- |
| Temperature(K) | ultimate elongation (%) |
| 293 | 14 |
| 573 | 11 |
| 623 | 10.5 |
| 673 | 11 |
| 723 | 13.5 |
| 773 | 14 |
| 873 | 21 |
| 923 | 24 |
| 973 | 21.5 |
| 1053 | 30 |
| 1173 | 30 |
| 1273 | 30 |
| 1373 | 30 |
| 1473 | 30 |

#### AIM1 and T91

The ultimate elongation of AIM1 alloy in FRED is given as:



where:  – ultimate elongation;

 – temperature (K).

#### SS316

For SS316 alloy, the equation of ultimate elongation is



where:  – ultimate elongation;

 – temperature (K).

### Cladding stress-strain curve parameters [Ckmn]

As shown in Figure 6, during the linear deformation part, the Hook’s law is used to describe the stress-strain curve:



where:  – effective stress (Pa);

 – Young’s modulus (Pa);

 – effective deformation.

The plasticity starts when the stress exceeds the yield stress (), and the nonlinear stress-strain curve is assumed to follow the Power law:



where:  – effective stress (Pa);

 – strength coefficient (Pa);

 – effective deformation;

*n* – strain hardening exponent.

At the yield point (), and are met simultaneously:



So the strain hardening exponent (*n*) is



At the burst point () of cladding, the following correlation is met:



So the strength coefficient () is



where:  – ultimate elongation.

According to and ,  and *n* can be obtained from the following iteration:

1) set the initial value:





2) calculate the value at the iteration step *i*:





3) calculate the relative tolerance at the iteration step *i*:



When the relative tolerance is smaller than the limited value which is set in the input file, the strength coefficient () and the strain hardening exponent (*n*) are obtained:





### Cladding failure criteria [Cfail]

Several failure criteria of claddings have been implemented in FRED code.

#### CRITERION 1: rupture criterion

This overstress criterion is applied to ss316 and t91 cladding:





where:  – effective stress (Pa);

 – radius of node *i* and node *i+1* (m);

 – number of radial clad nodes;

 – burst stress (Pa);

 – failure factor, when , the cladding is consider to be failed.

#### CRITERION 2: plastic instability criterion

This criterion is applied to ss316 cladding:





where:  – plastic strain;

 – radius of node *i* and node *i+1* (m);

 – number of radial clad nodes;

 – inner cladding radius and outer cladding radius (m);

 – ultimate elongation;

 – failure factor, when , the cladding is consider to be failed.

#### CRITERION 2: melting criterion

This criterion is applied to ss316 cladding:



where: – temperature(K);

 – melting point(K);

 – failure factor, when , the cladding is consider to be failed.

The cladding fails when any of the above conditions are fulfilled.

## Gap models

The gap heat transfer and inner pressure are simulated by FERD.

### Gap heat transfer [Gaphtc]

Open fuel-clad gap conductance depends on the gas mixture (helium + fission gases) thermal conductivity, gap width + roughness, radiation. When gap is closing, the dependence on contact pressure is added.

|  |  |
| --- | --- |
|  |  |

**Figure 7** Fuel-clad gap states

Therefore, the gap heat transfer is calculate by following model:



where:  – total conductance across the gap(W/m2-K);

 – gas conductance (W/m2-K);

 – conductance due to radiant heat transfer (W/m2-K);

 – conductance due to solid-solid contact (W/m2-K).

#### gas conductance

The gas conductance is described as:



where:  – thermal conductivity of gas mixtures (W/m-K);

 – gap distance (m);

 – relocation strain;

 – temperature jump distance (m).

The correlations used for thermal conductivity of gases are in the form of the equation:



where:  – thermal conductivity of gas (W/m-K);

 – gas temperature(K).

The values for A and B for each gas from MATPRO are given in Table 7.

Table 7 Constants used in gas thermal conductivity correlations

|  |  |  |
| --- | --- | --- |
| *Gas* | *A* | *B* |
| He | 2.639×10-3 | 0.7085 |
| Ar | 2.986×10-4 | 0.7224 |
| Kr | 8.247×10-5 | 0.8363 |
| Xe | 4.351×10-5 | 0.8618 |

The thermal conductivity of gas mixtures is given as:



where:  – thermal conductivity of the component *i* (W/m-K);

 – number of components in mixture;

 – mole fraction of component *i*.

The relocation strain is calculate by:



where:  – fuel rod linear power (W/m);

 – fuel burnup (MWd/kgU).

The jump distance is give as:



where:  – accomodation coefficient for helium as follow:



#### radiation conductance

The radiation conductance is described as:



where:  – Stefan-Boltzmann constant;

 – an emissivity function;

 – temperatures of fuel surface (K);

 – temperatures of cladding surface (K).

The emissivity function is defined as:



where:  – emissivity of fuel surface;

 – emissivity of cladding surface;

 – radius of fuel outer surface (m);

 – radius of cladding inner surface (m).

#### contact conductance

The contact conductance is described as:



where: , – thermal conductivity of fuel surface and cladding surface(W/m-K);

 – effective contact pressure (Pa);

 – Meyer hardness of the softer material (Pa);

,  – roughness of fuel surface and cladding surface (m).

### Gap pressure [Precal]

As shown in Figure 8, the fuel rod inner gas presents at different positions: rod plenum, fuel central hole, inside fuel pellet and the fuel-clad gap.



**Figure 8** Fuel rod inner gas

Gas pressure inside the fuel rod is calculated as follows:



where: P0, V0 – initial gas pressure and free volume at fuel rod manufacturing;

 – amount of fission gas released from the fuel in the free volume (moles);

 – the universal gas constant (J/mol-K).

Gas volume V and temperature T in the fuel rod free volume are determined taking into account the fuel rod deformation as follows:





where Vp, Tp – are the volume and temperature of gas in the gas plenum;

V1n , V2n , V3n – volume of gas in the central void, open porosity in fuel and fuel-clad gap, respectively, in axial slice n;

T1n , T2n , T3n – temperature of gas in the central void, open porosity in fuel and fuel-clad gap, respectively, in axial slice n;

NZ – number of axial calculational slices.

The gas temperature in the gas plenum is assumed equal to the average temperature of fuel and cladding surface.

## Coolant channel models

### Coolant specific heat [Baseir]

#### He

The value of specific heat for helium is



#### Pb-Bi

The value of specific heat for lead-bismuth coolant is



#### Pb

The value of specific heat for lead coolant is



#### Na

The value of specific heat for sodium coolant is



### Coolant temperature calculation [Baseir]

The calculation of coolant temperature using the relation:



where:  – coolant temperature at node (K),  is the node index;

 – inlet coolant temperature (K);

, –fuel rod power at node  and  (W);

 – flow rate (kg/s);

 – coolant specific heat (J/kg-K).

### Coolant thermal conductivity [Baseir]

#### He

The thermal conductivity of helium gas is given as:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### PbBi

The equation of thermal conductivity for PbBi:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

#### Pb

The equation of thermal conductivity for Pb:



where:  – thermal conductivity (W/m-K);

 – temperature (℃).

#### Na

The thermal conductivity of sodium coolant:



where:  – thermal conductivity (W/m-K);

 – temperature (K).

### Coolant density [Baseir]

#### He

The density of helium gas is given as:



where: – coolant density (kg/m3);

 – temperature (K);

 – coolant pressure (Pa);

 – universal gas constant = 8.314 J/K-mol.

#### PbBi

The density of PbBi is:



where: – coolant density (kg/m3);

 – temperature (℃).

#### Pb

The density of Pb using the relation:



where: – coolant density (kg/m3);

 – temperature (℃).

#### Na

The density of sodium using the relation:



where: – coolant density (kg/m3);

 – temperature (℃).

### Coolant heat transfer coefficient [Baseir]

The clad-to-coolant heat transfer coefficient is:



where: – heat transfer coefficient (W/m2-K);

 – thermal conductivity of coolant (W/m-K);

 – Nussel number;

 – hydraulic diameter of coolant channel (m).

#### He

In laminar flow, the Nusselt number of helium gas is consider as constant value, 4.36 [16]. While during the turbulent forced convection, the Nusselt number is calculating by Dittus-Boelter correlation [17]:



where:  – Nussel number;

 – Reynolds number;

 – Prandtl number.

The Reynolds number is given as:



where:  – coolant density (kg/m3);

 – coolant velocity (m/s);

 – hydraulic diameter of coolant channel (m);

 – hydrodynamic viscosity (Pa∙s).

The Prandtl number is given as:



where:  – coolant specific heat (J/kg-K);

 – hydrodynamic viscosity (Pa∙s);

 – thermal conductivity (W/m-K).

The hydrodynamic viscosity of helium gas:



where:  – temperature (K);

 – coolant density (kg/m3).

#### PbBi and Pb

For PbBi or Pb, the Nusselt number is given as:



where:  – Nussel number;

 – Peclet number.

The Peclet number is



where:  – coolant velocity (m/s);

 – hydraulic diameter of coolant channel (m);

 – thermal conductivity (W/m-K);

 – coolant density (kg/m3);

 – coolant specific heat (J/kg-K).

#### Na

The Nusselt number of sodium is obtained from K.Mikityuk [18] :



where:  – Nussel number;

 – Peclet number;

 – pitch to channel diameter ratio, =1.1.

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# Appendix A

APPENDIX A shows the steps of getting access to Merlin6 PSI cluster:

1. **Access request to merlin6**

The first step is to request the access to merlin6 cluster. It is necessary to report an incident at PSI service webpage by clicking the following link: <https://psi.service-now.com/psisp/?id=psi_report_new_incident&sys_id=797c79ebdbf20454d648f90532961982>

The user’s information has to be provided along with the following description:

Short description

[Merlin6] Access Request for user *lastname*\_*firstnameletter*

Long description

Dear HelpDesk,

I would like to request access to the Merlin6 cluster. This is my account information

\* Last Name: \*\*\*\*\*

\* First Name: \*\*\*\*\*

\* PSI user account: lastname\_firstnameletter

Please add me to the following Unix groups:

\* 'svc-cluster\_merlin6', ‘unx-ans’

Thanks,

\*\*\*\*\*\*

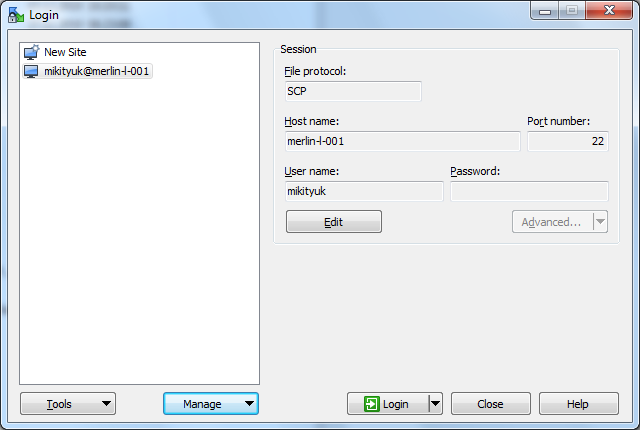
The approval process will not be long and the user will get the permission in the following hours. A confirmation e-mail will be received at the end of the request.

1. **Access to merlin6 disk space via WinSCP software (or similar)**

WinSCP can be installed using Software Kiosk installer on your Desktop:



After installation you should create a session using merlin-l-001 as a host name, 22 as a port number, you user PSI name and PSI password.



After Login you should have access to the Merlin disk space. You home directory is /psi/home/yourusername.

1. **Modify your .bashrc**

If you do not see .bashrc in your home directory, press: Ctrl+Alt+H which makes hidden files visible. Open .bashrc with the editor by pressing F4 (I specified Notepad++ as WinSCP F4 editor) and add the following lines at the end of the file:

#get AFS cridentials

aklog

#load intel fortran compiler

module load intel/19.3

You can add also aliases as you like, e.g.:

#aliases

alias fast="cd /afs/psi.ch/project/fast\_lrs"

alias home="cd /psi/home/yourusername"

alias ans="cd /data/project/general/ans"

The .bashrc will be properly updated by executing “source .bashrc” in the command window or by restarting the session.

After getting the AFS credentials you can see AFS disks in WinSCP and easily copy files from Merlin to AFS and back.

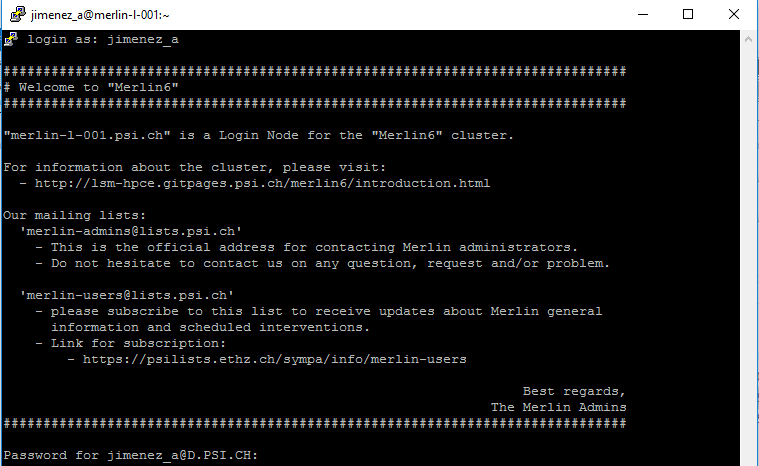
1. **Access to merlin6 cluster via PuTTY software**

Once the access to merlin6 is approved, the software PuTTY from Software Kiosk has to be employed in order to access and to work in the cluster.

Host Name: merlin-l-001

Port: 22

This is how the merlin6 main page looks like:



Besides, for getting information about downtimes and updates of Merlin, see following link:

<https://lsm-hpce.gitpages.psi.ch/merlin6/faq.html#how-do-i-get-information-about-downtimes-and-updates>