

FRED: Fast reactor fuel behaviour code

Version: 1.1.0 (20241115)

Modifications

1.0.0

Initial version

1.0.1

Fiel FRED_.f90 with the old FRED code was removed

1.1.0 (20241115)

1. Fortran files were re-organized as follows:

- main.f90: main driver
- FRED.f90: DAE residual function, all models, Equations-of-State and auxiliary functions.
- globals.f90: declaration of all global variables

2. Restart was introduced. Now all variables and derivatives are stored in a separate rstfrd file for every timestep. The new input card allows specifying from which rstfrd to restart.

3. New criteria for the root function were introduced. The new input card allows specifying the exact times which the solver should make. To be tested.

4. MOX fuel swelling model was modified. The new input card allows specifying the multiplier for the swelling rate.

5. Material properties for stainless steel t91 were added.

6. New example of FRED input file was added.

1. Summary

Open-source Fortran code uses the SUNDIALS library for numerical modelling of base irradiation of a fast reactor fuel pin, accounting for fuel and clad heat transfer, fuel and clad stress-strain conditions, fuel and clad thermal expansion and creep, fuel swelling and fission gas release, evolution of inner gas pressure and composition as well as evolution of fuel-clad gap conductance.

Algebraic and ordinary differential equations are solved by finite-difference method on a structured r-z cylindrical mesh using the SUNDIALS library.

As the input, FRED takes time-dependent axial profile of power density assuming flat power distribution over the radius, time-dependent axial profile of clad outer temperature, as-manufactured fuel and clad dimensions, mesh specification, as well as several constants for material properties and flags to activate specific models.

The typical dataset of the calculational results includes time-dependent radial and axial maps of fuel and clad deformations, stresses, and temperatures; axial profiles of fuel-clad gap conductance, contact pressure, burnup, fuel and clad dimensions.

Available materials:

- Fuel: MOX.
- Clad: AIM1 stainless steel, T91 stainless steel.
- Bonding: helium, xenon, krypton.
- Inner gas: helium, xenon, krypton.

2. Installation

First you need to install the SUNDIALS library <https://computing.llnl.gov/projects/sundials>:

1. Create `INSTDIR` and `BUILDDIR`
2. Download the last version of IDA, e.g. `ida-7.0.0` archive from <https://computing.llnl.gov/projects/sundials/sundials-software> and unpack it in the `BUILDDIR` directory using `tar -zxvf ida-7.0.0.tar.gz`
3. In `BUILDDIR` directory perform three commands:

```
cmake -DCMAKE_INSTALL_PREFIX=/path/to/sundials/INSTDIR
-DEXAMPLES_INSTALL_PATH=/path/to/sundials/INSTDIR
-DBUILD_FORTRAN_MODULE_INTERFACE=ON
./ida-7.0.0
```

```
make
```

```
make install
```

Then install the code itself:

1. Download the last version of the code from github and unpack the archive.
2. In `Makefile` file specify the path to SUNDIALS installation directory and the path to the FORTRAN compiler (`gfortran`).

3. Perform `make` to generate executable and run: `./FRED`
4. Post process the results (see Section “Postprocessing script `postprocess.py`”)

3. Input file specification

The input file should have name `fred.inp`. It consists of cards described below.

Comment (*)

Asterisk `*` at the first position shows that the card is a comment.

Options (000001)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           OPTIONS CARD
*-----1-----2-----3-----4-----5-----6-----7-----
000001      FGR
000001      FUEL_CREEP
000001      FUEL_SWEL          1.0
000001      CLAD_CREEP
000001      FUEL_RELOC
000001      NOMECH
```

Every card activates a specific model: fission gas release (`FGR`), fuel creep (`FUEL_CREEP`), fuel swelling (`FUEL_SWEL`) and a multiplier of the swelling rate (tuning factor), clad creep (`CLAD_CREEP`), fuel relocation (`FUEL_RELOC`). The card with the keyword `NOMECH` allows to switch of the whole mechanical calculations.

Initial temperature (000002)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           INITIAL TEMPERATURE CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      tem0
000002      668.0
```

At time zero all temperatures are set equal to the initial temperature (K) specified by this card.

Axial division (000003)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           INITIAL AXIAL DIVISION CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      dz0      nz
000003      0.05     17
```

The code uses a uniform axial nodalization. The axial division card specified the height of the axial layers (m) and the number of the axial layers.

Fixed time (000004)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           FIXED TIME CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      ftime
000004      86400.0
```

The user can instruct the solver to reach exact times (up to 50 cards).

Fuel (100001)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           FUEL CARD
```

```

*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      fmat      fden      pucont    rfi      rfo      ruff      stoch      nf
100001      mox       10410.    0.45     1.0E-3    2.71E-3    3.0E-6    2.0        22

```

The card specifies the fuel material (only `mox` is available for the current version), as-fabricated fuel density (kg/m³), plutonium weight fraction (kg/kg), inner and outer radii of the fuel pellet (m), fuel outer surface roughness (m), initial stoichiometry of the fuel, and number of the radial nodes.

Gap (100002)

```

*-----1-----2-----3-----4-----5-----6-----7-----
*          GAP CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      gmat      dgap      pin      vpl
100002      he       115.0E-6  0.1     1.455E-5

```

The card specifies the gap material (only `he` is available for the current version), as-fabricated fuel-clad gap width (m), as-fabricated inner gas pressure (MPa), and gas plenum volume (m³).

Clad (100003)

```

*-----1-----2-----3-----4-----5-----6-----7-----
*          CLADDING CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      cmat      rco      roc0     rufc      nc
100003      aiml     3.275E-3  7900.   1.0E-6    3

```

The card specifies the cladding material (`aiml`, which is 15-15Ti stainless steel, and `t91` stainless steel are available for the current version), as-fabricated outer clad radius (m) and density (kg/m³), as well as number of radial nodes in the cladding.

Time (200000)

```

*-----1-----2-----3-----4-----5-----6-----7-----
*          TIME CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      tend      dtout     hmax
200000     3.494398E8  86400.   3600.

```

The card specifies the final time (s), output time step (s) and maximum time step (s).

Clad outer temperature vs time table (200001)

```

*-----1-----2-----3-----4-----5-----6-----7-----
*          CLAD OUTER TEMPERATURE VS TIME TABLE
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      time      tc01     tc02     tc03     tc04     tc05     tc06
200001      0.0       668.0    668.0    668.0    668.0    668.0    668.0
200001      3600.0    660.75   674.50   686.00   698.25   711.70   725.80

```

Up to 50 cards can be used to specify the evolution of the axial profile of outer cladding temperature (K) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the clad outer temperature should be equal to the initial temperature specified in card 000002.

Power density vs time table (200002)

```

*-----1-----2-----3-----4-----5-----6-----7-----
*          POWER DENSITY CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      time(s)   qv1      qv2      qv3      qv4      qv5      qv6
200002      0.0       0.0      0.0      0.0      0.0      0.0      0.0
200002      3600.    1.11095E9 1.26272E9 1.40308E9 1.54105E9 1.63463E9 1.70308E9

```

Up to 50 cards can be used to specify the evolution of the axial profile of power density (W/m^3) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the power density should be equal to zero.

Fuel creep rate law constants (200003)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           FUEL CREEP RATE LAW CONSTANTS
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      C1          C2          C3
200003      1.0E-39     1.0          0.0
```

The card specifies three constants used in the creep rate law: $\text{ECR} = C1 * \text{SIG}^{**}C2 * \exp(-C3 / (R * T))$, where SIG is the stress (MPa), R the universal gas constant (J/mol-K) and T the temperature (K).

Fuel stoichiometry vs fuel burnup table (200004)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           FUEL STOICHIOMETRY VS BURNUP
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      bup          stoich
200004      0.0          2.0
200004      100.         2.0
```

Up to 50 cards can be used to specify the dependence of fuel stoichiometry (-) on burnup (MWd/kg).

Coolant pressure (200005)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           COOLANT PRESSURE CARD
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      press
200005      0.2
```

The card specifies the coolant pressure (MPa) assumed constant. This is boundary condition.

Gas plenum temperature vs time table (200006)

```
*-----1-----2-----3-----4-----5-----6-----7-----
*           GAS PLENUM TEMPERATURE VS TIME TABLE
*-----1-----2-----3-----4-----5-----6-----7-----
*crdno      time          tple
500001      0.0           668.0
500001      3600.         660.75
```

Up to 50 cards can be used to specify the evolution of plenum temperature (K) with time (s). This is boundary condition. Note that to avoid convergence problems, at time zero the gas plenum temperature should be equal to the initial temperature specified in card 000002.

4. Output file **outfrd**

The main output file is the ASCII file generated at every output time step with the name **outfrdXXXXXXXXXXXX**, where **XXXXXXXXXXXX** is the time step number. The file contains the following information:

time (s)	Current time
time (d)	Current time

rof0 (kg/m3)	Initial fuel density
figgen (cm3)	Volume of generated fission gas

fgrel (cm3)	Volume of released fission gas	
fgrel (%)	Fission gas release, i.e. released-to-generated fission gas ratio	
gpres (MPa)	Inner gas pressure	

z (m)	Coordinates of the axial nodes	
tfin (C)	Axial profile of the inner fuel temperature	
tfout (C)	Axial profile of the outer fuel temperature	
tcin (C)	Axial profile of the inner cladding temperature	
tcout (C)	Axial profile of the outer cladding temperature	
rfi (m)	Axial profile of the inner fuel radius	
rfo (m)	Axial profile of the outer fuel radius	
rci (m)	Axial profile of the inner cladding radius	
rco (m)	Axial profile of the outer cladding radius	
dzf (m)	Axial profile of the axial fuel layer heights	
dzc (m)	Axial profile of the axial cladding layer heights	
reloc (-)	Axial profile of fuel relocation in fractions of the initial gap	
qv (W/m3)	Axial profile of power density	
ql (W/cm)	Axial profile of linear heat generation rate	
ql2 (W/cm)	Axial profile of linear heat generation rate with account for axial strain	
bup (MWd/kg)	Axial profile of fuel burnup	
gap (m)	Axial profile of fuel-clad gap	
gapth (m)	Axial profile of fuel-clad gap with accommodation distance and fuel relocations	
hgap (W/m2K)	Axial profile of fuel-clad gap conductance	
hgap1 (W/m2K)	Axial profile of the conduction component of fuel-clad gap conductance	
hgap2 (W/m2K)	Axial profile of the radiation component of fuel-clad gap conductance	
hgap3 (W/m2K)	Axial profile of the contact component of fuel-clad gap conductance	
ajump (m)	Axial profile of the accommodation distance of fuel-clad gap	
gask (W/m-K)	Axial profile of the fuel-clad gap conductance	
pfc (MPa)	Axial profile of the fuel-clad contact pressure	

r (m)	Coordinates of the radial nodes	
temperature (C)	iz: 1	Radial profile of temperature
...		
sig h (MPa)	iz: 1	Radial profile of hoop stress for every axial level
...		
sig r (MPa)	iz: 1	Radial profile of radial stress for every axial level
...		
sig z (MPa)	iz: 1	Radial profile of axial stress for every axial level
...		
eps h total (%)	iz: 1	Radial profile of hoop total strain for every axial level
...		
eps r total (%)	iz: 1	Radial profile of radial total strain for every axial level
...		
eps z total (%)	iz: 1	Radial profile of axial total strain for every axial level
...		
eps h creep (%)	iz: 1	Radial profile of hoop creep strain for every axial level
...		
eps r creep (%)	iz: 1	Radial profile of radial creep strain for every axial level
...		
eps z creep (%)	iz: 1	Radial profile of axial creep strain for every axial level
...		
eps thermal lin (%)	iz: 1	Radial profile of linear thermal expansion strain for every axial level
...		
eps swell vol (%)	iz: 1	Radial profile of volumetric swelling strain for every axial level
...		

5. Postprocessing script `postprocess.py`

For postprocessing:

1. Create virtual environment:

```
python3 -m venv venv_fred
```

2. Activate it:

```
source venv_fred/bin/activate
```

3. Update pip

```
pip install --upgrade pip
```

4. Install libraries:

```
python -m pip install python-pptx  
python -m pip install -U matplotlib
```

5. Run the script:

```
python postprocess.py
```

The script reads the output files `outfrd` which should be in the working directory and creates two PowerPoint files: `plot-bup.pptx` and `plots-time.pptx`. The first contains the plots of key variables as a function of time and the second one—as a function of burnup.

At the beginning of the script the user should provide three values which are explained by the comments:

```
#axial level for output  
jz = 8  
#number of fuel radial nodes  
nf = 22  
#number of clad radial nodes  
nc = 3
```