Temperature coefficients of reactivity in Molten Salt Reactor Experiment calculated with direct method using Serpent 2 Monte Carlo code

Monte Carlo Course at KTH Stockholm taught by Assoc. Prof. Jan Dufek, final project

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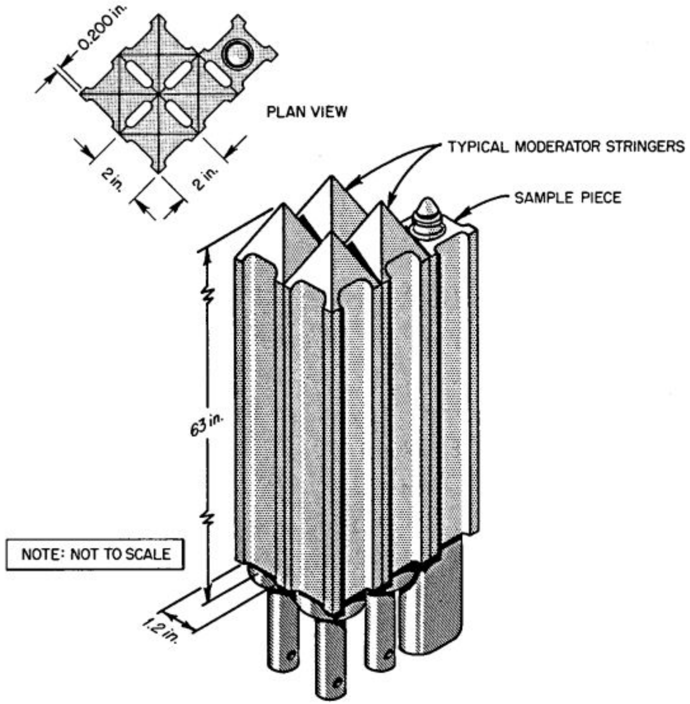
Table of Content

1) Problem Statement

- The temperature coefficients of reactivity are evaluated for the Molten Salt Reactor Experiment (MSRE) considering different
  - materials (fuel salt, graphite moderator, vessel)
  - effects (thermal expansion, Doppler, moderator effect = thermal scattering)
- Assumptions:
  - Zero flow velocity
  - Spatially constant temperature for materials and effects separately
  - Control rods were kept at 900 K

- BENCHMARK EVALUATION OF REACTIVITY EFFECTS AND REACTIVITY COEFFICIENTS IN THE MOLTEN SALT REACTOR EXPERIMENT, 2021
  Dan Shen and Massimiliano Fratoni, University of California, Berkeley Department of Nuclear Engineering, Berkeley CA 94720-1730

2) MSRE Core Design



- ORNL-TM-0728 MSRE Design & Operations, Part I
- https://tcr.ornl.gov/or14/

2) MSRE Core Design

Power	8 MWth
Fuel	57 LiF - 29.1 BeF_3 - 5 ZrF_4 - 0.9 UF_4 (mass %)
Core diameter	137 cm (graphite)
Height	163 cm (graphite)
Average coolant temperature:	around 900 K

- ORNL-TM-0728 MSRE Design and Operations Report, Part I
- Fuel Type C, Table 3.2 in ORNL-TM-0730 MSRE Design and Operations Report, Part III

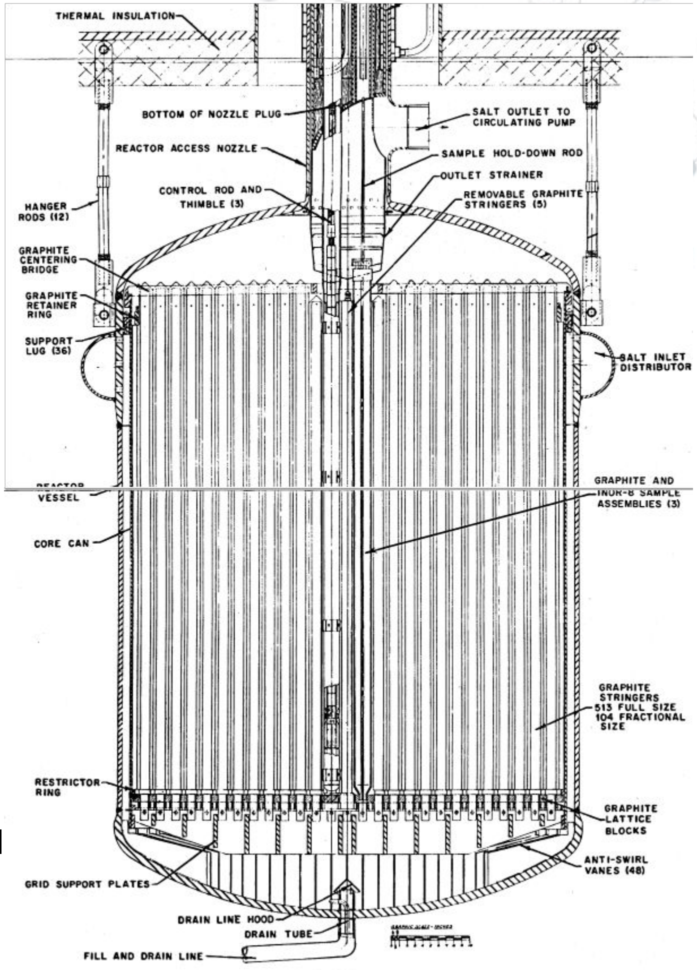
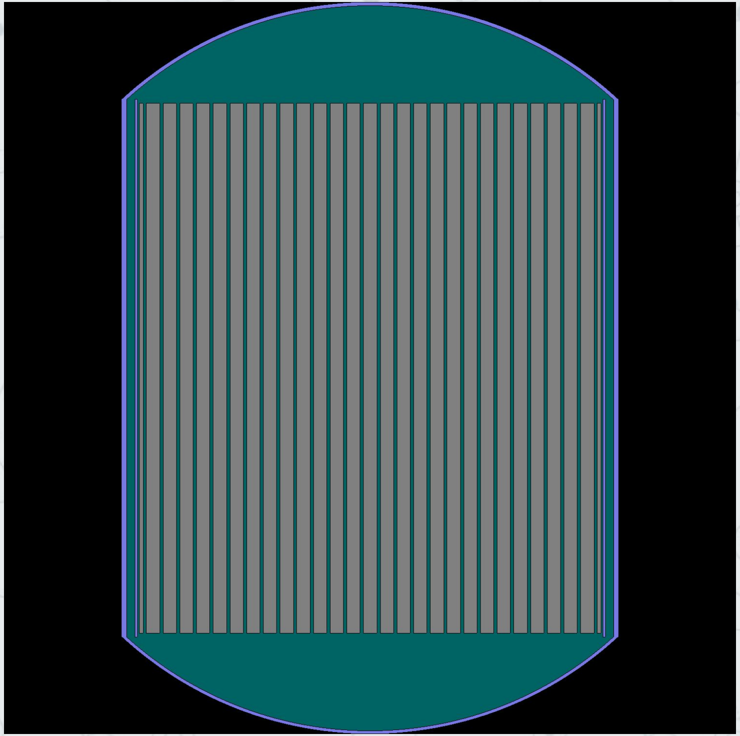
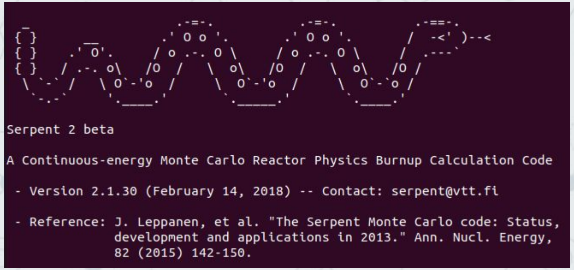
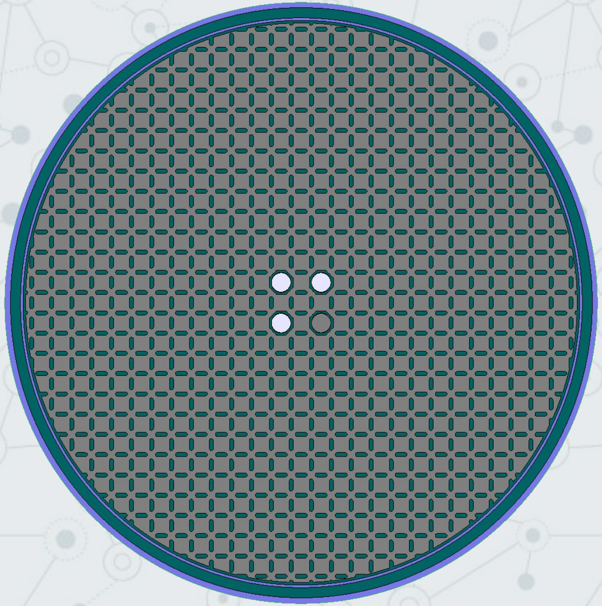


Fig. 5.4.
CROSS SECTION
MSRE REACTOR VESSEL AND ACCESS NOZZLE

2) MSRE Core Design: Serpent 2







- Master Thesis, Matheusz Pater, Multiphysics simulations of Molten Salt Reactors using the Moltres code, 2019

3) Method: Definition of reactivity & temperature coefficient

$$\rho = \frac{k-1}{k}$$

$$\sigma_\rho = \frac{\sigma_k}{k^2}$$

$$\alpha = \frac{1}{k}\frac{\partial k}{\partial T} = k\frac{\partial \rho}{\partial T}$$

$$\alpha \approx \frac{1}{k_1}\frac{k_2 - k_1}{\Delta T}$$

$$\sigma_\alpha = \sqrt{\left(\frac{\partial \alpha}{\partial k_1}\right)^2 \sigma_{k_1}^2 + \left(\frac{\partial \alpha}{\partial k_2}\right)^2 \sigma_{k_2}^2}$$

3) Method: Reactivity depends on multiple temperatures

$$\rho = \rho(T_0, T_1, T_2, T_3, T_4, T_5)$$

$$\frac{d\rho}{dT} = \sum_{i=0}^{5} \frac{\partial \rho}{\partial T_i}$$

T_0	Doppler effect in fuel salt
T_1	Doppler effect in other materials
T_2	Thermal expansion and density in graphite
T_3	Thermal expansion and density in steel
T_4	Density in fuel salt
T_5	Thermal scattering in graphite

3) Method: Linear thermal expansion coefficient

$$\gamma(T) = \frac{1}{l}\frac{dl}{dT} = \frac{d}{dT}\ln(l)$$

material	$\gamma/10^{-6}\mathrm{K}^{-1}$
graphite	$5.52+0.001\cdot T$
INOR-8 (21°C-982.2°C)	15.0
fuel salt	78

$$l(T+\Delta T) = l(T)e^{\int_T^{T+\Delta T}\gamma(T)dT}$$

$$l(T+\Delta T) \approx l(T)(1+\gamma\Delta T)$$

- R. Robertson, “Conceptual design study of a single-fluid molten-salt breeder reactor,” 1971.
- WASH-1222 U. D. of Reactor Development and Technology, “Evaluation of the molten salt breeder reactor,” 1972.

3) Method: Volumetric expansion and density change

$$V(T + \Delta T) = V(T)(1 + \gamma \Delta T)^3$$

Mass is unchanged:

$$M = \rho(T)V(T) = \rho(T + \Delta T)V(T + \Delta T)$$

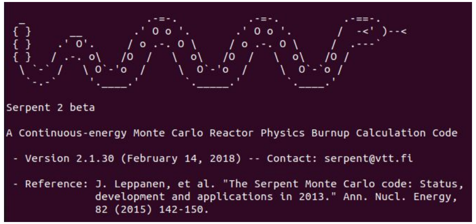
$$\rho(T + \Delta T) = \frac{\rho(T)}{(1 + \gamma \Delta T)^3}$$

3) Method: Implementation in Python

step01_generate_input_files.py

step02_run_input_files.py

step03_read_output_files.py

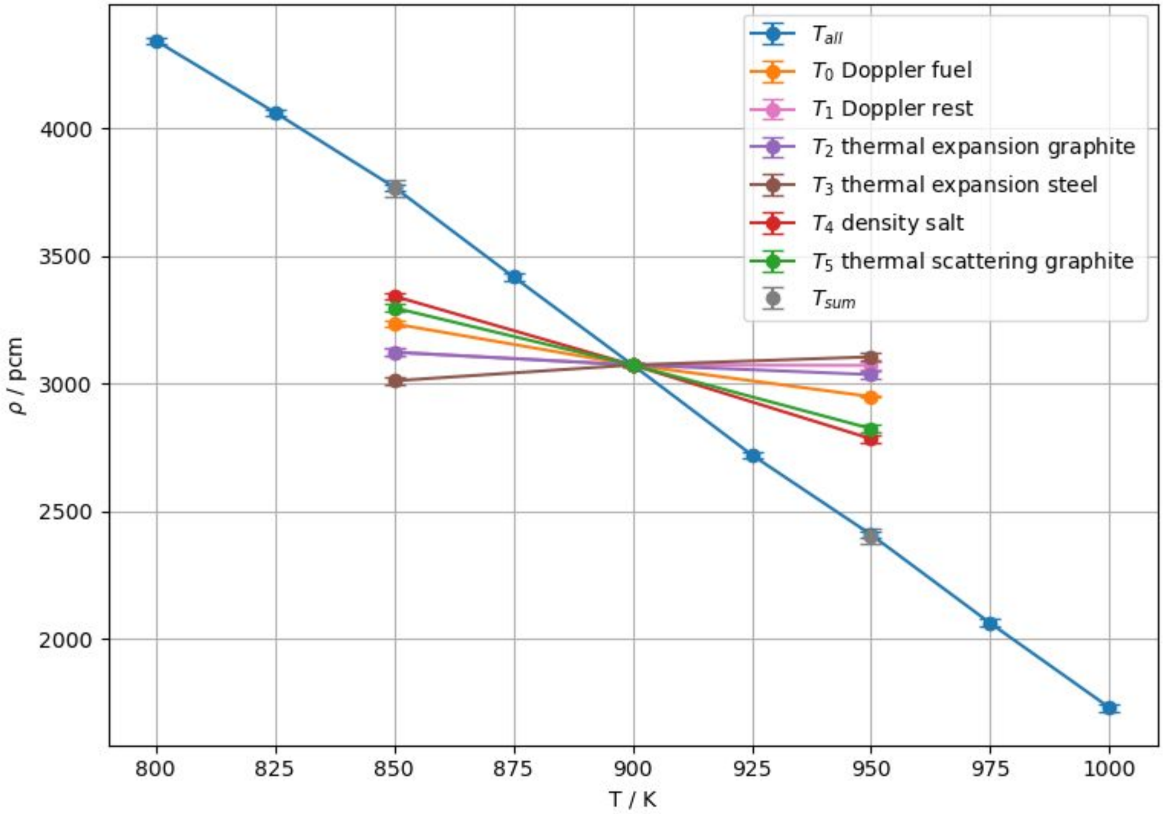


- https://github.com/MartinTa/MSRE

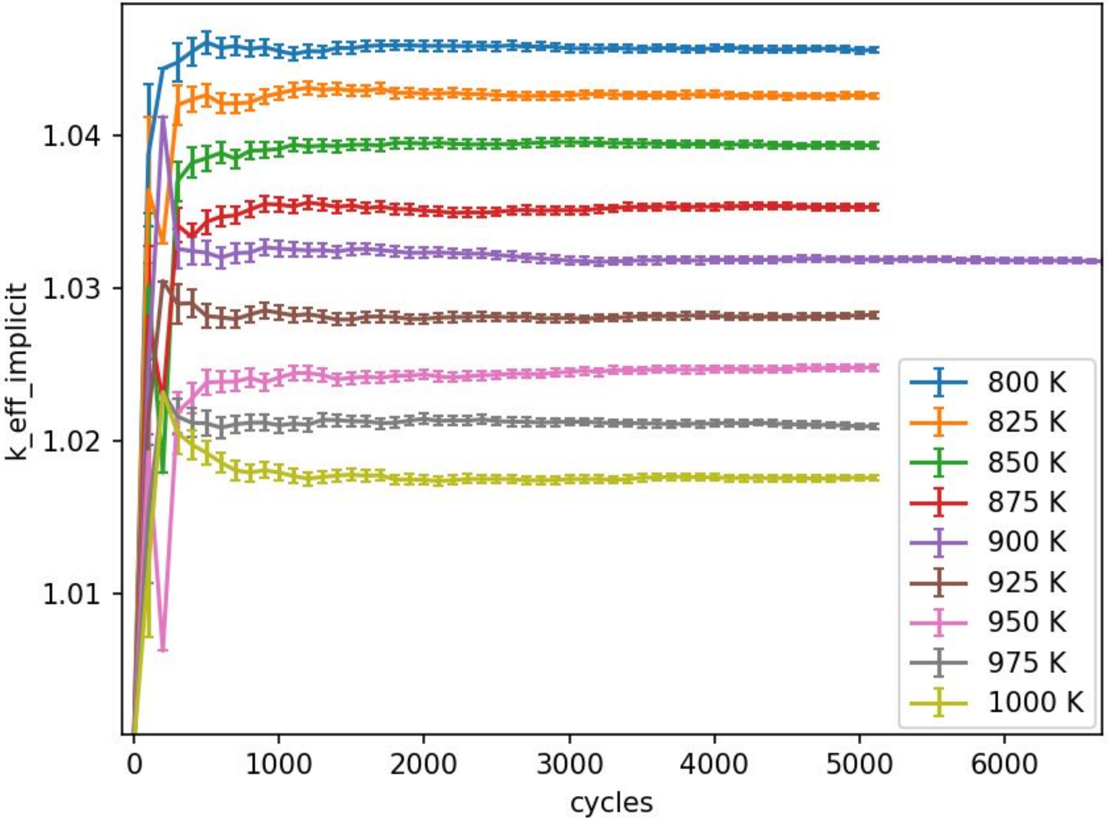
3) Method: How to run many serpent simulations

```python
# T0 / K ... nuclide temperature for doppler effect in fuel salt
# T1 / K ... nuclide temperature for doppler effect in all other materials
# T2 / K ... used for thermal expansion and density change of graphite
# T3 / K ... used for thermal expansion and density change of steel (hastalloy)
# T4 / K ... used for density change in fuel salt
# T5 / K ... thermal crosssection library for graphite
def GetInputStr(T0,T1,T2,T3,T4,T5):
    graphite_length_scale_factor = np.exp(5.52E-6*(T2-273.15)+0.001E-6/2*(T2-273.15)**2)
    steel_length_scale_factor = 1 + 15E-6*(T3-273.15-21)
    fuel_length_scale_factor = 1 + 78E-6*(T4-648.88-273.15) # reference density given at 1200 F
    enrichment = 0.33 # 0.29 gives criticality

    graphite_density_scale_factor = 1/graphite_length_scale_factor**3
    steel_density_scale_factor = 1/steel_length_scale_factor**3
    fuel_density_scale_factor = 1/fuel_length_scale_factor**3
    #print(f'fuel density scale factor = {fuel_density_scale_factor:.8f}')

    T0_marker = GetTemperatureMarker(T0)
    T1_marker = GetTemperatureMarker(T1)
    input_file_str = """% --- MSR cluster ------------------------------------------
set title "MSR2G - partially - enriched -U-full - core "

%% --- get the stringer unit cell (graphite rod)
surf 11 inf
surf 12 inf
surf 13 inf
surf 14 inf
surf 15 inf
cell 111 2 fuel -11
cell 112 3 moder -12
cell 113 4 tank -13
cell 114 5 ctrlPois -14
cell 115 6 air -15

% --- Single unit cell
% 4 bounding planes of stringer
surf 1 px {:.5f}""".format(-2.54*graphite_length_scale_factor) + """
```

4) Results and Discussion



4) Results and Discussion: convergence plot



set pop 10000 5000 200

4) Results and Discussion

Temperature Coefficients and sum of individuals	**alpha_low (pcm/K)**	**alpha_high (pcm/K)**
Doppler effect in fuel salt	-3.33 +/- 0.28	-2.56 +/- 0.10
Doppler effect in other materials	-1.05 +/- 0.28	-0.04 +/- 0.28
Thermal expansion and density in graphite	-1.03 +/- 0.28	-0.78 +/- 0.28
Thermal expansion and density in steel	1.28 +/- 0.28	0.66 +/- 0.28
Density in fuel salt	-5.58 +/- 0.28	-5.95 +/- 0.30
Thermal scattering in graphite	-4.63 +/- 0.28	-5.14 +/- 0.30
Sum of total of Temperature Coefficient	-14.35 +/- 0.69	-13.80 +/- 0.65
Direct total using Serpent 2	-14.48 +/- 0.28	-13.63 +/- 0.30

Conclusion

	alpha_low (pcm/K)	alpha_high (pcm/K)
Direct total α	-14.48 +/- 0.28	-13.63 +/- 0.30
Measured total α	-13.14 +/- 0.36	
Doppler + density of fuel	-8.91 +/- 0.39	-8.51 +/- 0.31
Measured Doppler + density of fuel	-8.8 +/- 4.1	

- N. Haubenreich, J. R. Engel, B. E. Prince, and H. C. Claiborne, “Experience with the molten-salt reactor experiment. Nuclear Applications and Technology, 8(2):118-136, 1970. arXiv: https://doi.org/10.13182/NT8-2-118,doi:10.13182/NTB-2-118

“

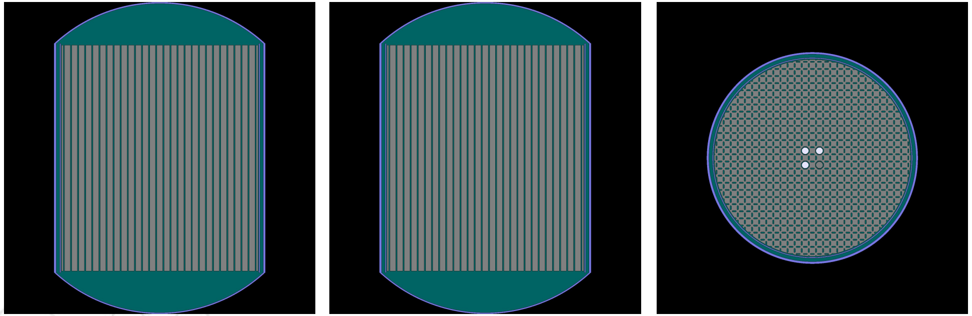
The most important fact of all
is the fact of your own ignorance.

(Philosophy and Fun of Algebra
by Mary Everest Boole)

Extra slides: How to not run Serpent

Neutron ended up far away (program terminated),

even though “outside” cell was defined as well as vacuum boundary condition. Geometry from all 3 plots looked good. How is that possible?



```
Tracking error: infinite loop (after 1000000 cycles)

Particle type : neutron

Collision = 651544633
(x,y,z)    =  3.26381E+06  1.40039E+07  1.38956E+07
(u,v,w)    =  1.63221E-01  7.00330E-01  6.94908E-01
E          =  1.81455E+00
Emin       =  1.00000E-11
Emax       =  2.00000E+01
material   =  void / undefined
totxs      =  0.00000E+00
majorant   =  2.62312E-01

Lost particles: 0

Checking geometry errors (this may fail)...

No geometry errors, but infinite loop may occur if
particle energy is outside the range of most cross
section libraries and collision probability becomes
```

Extra slides: How to not run Serpent