Advanced Depletion Extension for Reprocessing (ADER) for SERPENT 2

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Outline

- The problem
- The solution
  - Chemical composition control
  - REDOX potential control
  - Removal
  - Reactivity control
- Questions

The Problem

- With renewed interest in molten-salt reactors comes a need to be able to model the fuel and salt evolution over time in these reactors
- Previous attempts to address this problem relied on code to code coupling or system specific modifications to existing codes [2][1].
- No chemistry control
- No REDOX control

The Solution

- Modify SERPENT-2 to allow a user to specify for any material…
  - Relationships between groups of chemical, elemental, or isotopic constituents
  - Ranges of compositions for materials
  - Continuous and discreet removal and feed of chemicals, elements and isotopes
  - The average oxidation state as well as the average oxidation state of elements
  - Compositions of feed materials to be used as makeup material, or fuel, if needed to satisfy other constraints
  - Ranges of acceptable reactivity for a system as well as the “reactivity weight”

Chemistry/Composition Control

- This portion of the modification allows for complete or partial control of a material's makeup.
- Material -> Group(s) -> Element(s) -> Isotope(s)
- Material
  - ➢ $Group_i$[min – max]
    - ➢ $Element_{i,j}$[min – max]
      - ➢ $Isotope_{i,j,k}$[min – max]
- Groups in materials may have variable ratios with other groups
  - – $Group_a$ [min – max] : $Group_b$

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Chemistry/Composition Control

Group 001	Group 002	Group 003	Group 004
F 0.57	U [0.2 – 0.25] U-233 [0.2 – 0.3] U-238 [0.7 – 0.8]	Th 1.0	F 1.0
Li 0.29	F [rem]		
Be 0.14			

Material: Salt
Group 001 [0.33 , 0.66]
Group 002 [0 , 0.42]
Group 003 [0.20 , rem]
001 [1 , 3] : 002
004 [3 , 4] : 003

Chemistry/Composition Control

- Linear optimization is used to find the ratios and ranges which will satisfy the constraints
- Users may pick the optimization target though a default is provided

Chemistry/Composition Control

Feed 100 - C	Feed 200 - C	Feed 300 - D	Removal 400 - C	Removal 500 - D
F 0.57	U 0.2 U-233 1.0	Th 0.2	F 0.57	U 1.0
Li 0.29 Li-6 0.0001 Li-7 0.9999	F 0.8	F 0.8	Li 0.29 Li-6 all Li-7 rem	
Be 0.14			Be 0.14	

Chemistry/Composition Control

- Per material, an element or isotope may be specified to be completely accounted for in the groups assigned to said material
  - H – no
  - He – no
  - ….
  - U – yes
  - ….
  - Am - no
- All elements and isotopes in a material DO NOT have to be a part of a group

REDOX Potential Control

- Not actually REDOX – oxidation state control
- Inputs:
  - Material: [Min Oxidation – Max Oxidation]
  - Elements: Oxidation , weight

R - Feed 100 - C	R - Feed 200 - D	R - Removal 400 - C
F 1.0	Li 1.0 Li-6 0.0001 Li-7 0.9999	F 0.57
		Li 0.43 Li-6 all Li-7 rem

Removal

- Continuous proportional removal will be supported much in the same way it was in SERPENT-2.1.24; except each material may have its own
- Additionally, discreet and continuous removal based on groups

Removal 900 - C	Removal 800 - D
Np 0.2	U 0.2 U-238 – 0.8 U-233 – 0.2
F 0.8	F 0.8

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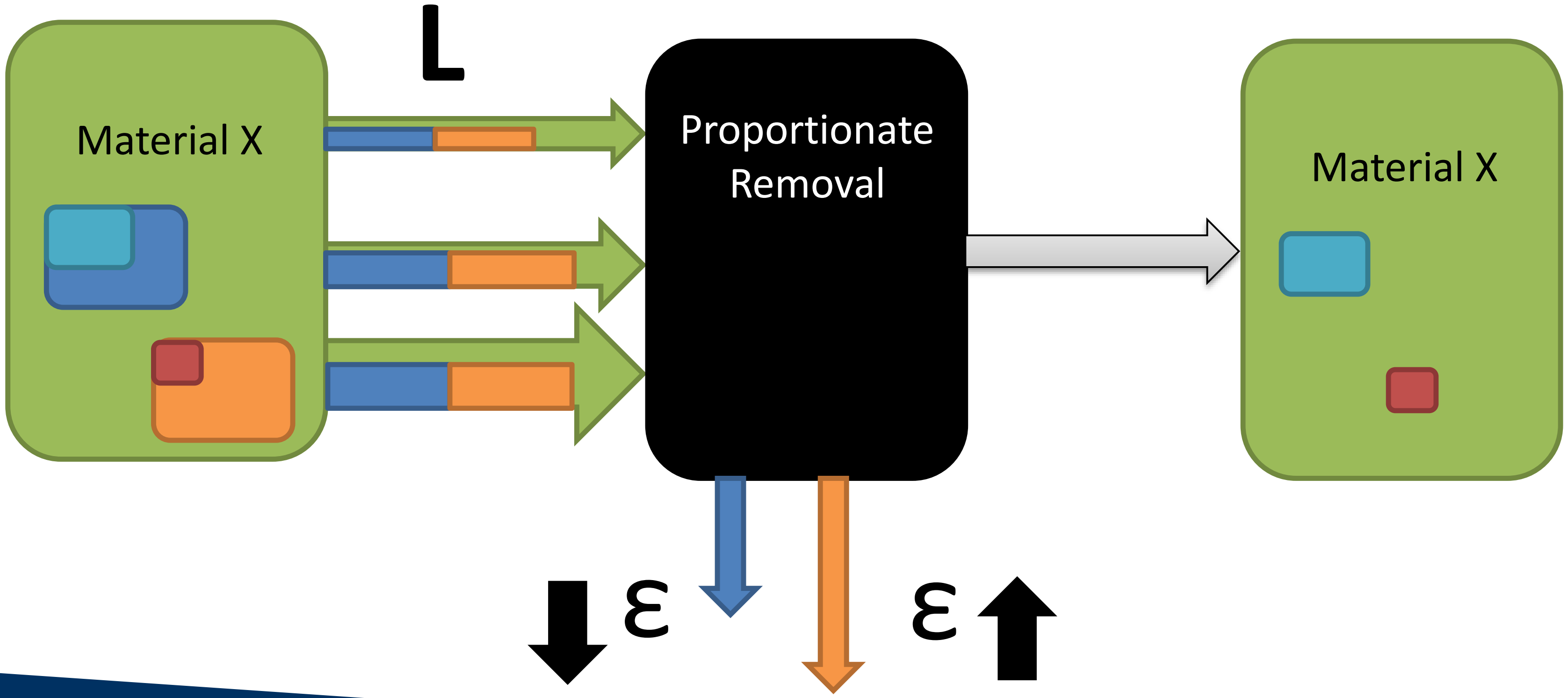
Removal

- If time allows, removal rate search feature



Reactivity Control

- k_{eff} [min – max]
- $k_{eff} \approx p_L \times \frac{\sum_n^N \nu^n \Sigma_f^n}{\sum_n^N \Sigma_a^n}$
- $k_{eff} \approx p_L \times \sum_m^M \left(\frac{\sum_n^N \nu^{m,n} \Sigma_f^{m,n}}{\sum_n^N \Sigma_a^{m,n}} \times w_m \right)$

Reactivity Control

ρ - Feed 100 - C	ρ - Feed 200 - D	ρ - Removal 400 - C
U 0.2 U-233 0.0495 U-238 0.9505	Pu 0.3333 P-239 0.23 P-240 0.77	U 1.0 U-233 1.0
F 0.8	F 0.6667	

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References

1. Aufiero, M., A. Cammi, C. Fiorina, J. Leppänen, L. Luzzi, and M. E. Ricotti. “An Extended Version of the SERPENT-2 Code to Investigate Fuel Burn-up and Core Material Evolution of the Molten Salt Fast Reactor.” *Journal of Nuclear Materials* 441, no. 1 (2013): 473–86.
2. Trellue, Holly, and David Poston. “User’s Manual, Version 2.0 for Monteburns, Version 5B.” Los Alamos Scientific Laboratory of the University of California, September 1, 1999.