The code development for the analysis of molten salt reactor

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Brief introduction of NECP lab. from XJTU, China

- One of the earliest teaching & researching group on reactor physics in Chinese university since 1958
- Establishing the NECP (Nuclear Engineering Computational Physics) lab. in 2004
- 38 teachers, graduate students, post-doctors now are studying and working in the lab.
- Two main aspects are focused on in recent years
  - The deterministic numerical methods for neutron transport/diffusion solution and resonance calculation
  - The core analysis and evaluation on the PWRs and new generation reactors
• The deterministic numerical methods
  ➢ Method of Characteristic (MOC), Nodal Method, etc. for neutron transport/diffusion
  ➢ Sub-group/Hyper-fine group/Continuous energy methods for resonance
    – The 1st lattice code for PWR in China (TPFAP in 1990s, cooperating with NPIC)
    – the neutronics-thermal-hydraulic coupling analysis codes for SCWR design in NPIC and CGNPC (neutronics part)
    – the core analysis code for the conceptual design of solution reactor and pebble-bed type PWR in NPIC
    – the code analysis code for the operation support of HFETR in NPIC
• Core analysis of reactors (on the view of neutronics)
  - Reactors: SCWR, FR (including long-life reactor), etc.
  - Sub-critical system: ADS and fusion-fission hybrids
The code development for the analysis of MSR

I. Background
II. Our activity
III. Verifying and Validation
IV. Conclusion
Molten salt reactor (MSR) an attractive option in the future development of nuclear energy

- High safety performance (Inherent safety)
- Flexibility in the nuclear fuel cycle
- High efficiency in utilizing the resources
- Non-proliferation
- Potential high economy due to the high thermoelectric efficiency

MSR on the way

- Before 1970: ARE, MSRE, MSBR
- After 2000: MOSART (Russia, 2001), TMSR (France, 2004), etc.
- Thorium-based molten salt reactor (China, 2011)
Current R&D activities on MSR

- Conceptual design proposal and fuel cycle analysis
- Materials, Facilities and Experiments
- Numerical simulation and analysis (Neutronics, T-H, Systemic Safety...)
- Others

The code developments

- Main results of the reactor performance and fuel cycle are generated from the numerical simulation
- Basic tool for the safety evaluation
- The codes are not so commonly shared (even of purchase) in the worldwide
Content

I • Background
II • Our activity
III • Verifying and Validation
IV • Conclusion
The composition of a core analysis code

Challenges (on neutronics only):

- Nuclear data, especially the data of thorium
- Neutron transport/diffusion solution (…)
- Depletion analysis (reprocessing online)
- Kinetics (Delayed neutron emission in the loops)

1. Power distribution
2. Change of density (fuel…) & Temperature distribution (fuel, moderator…)
Neutron transport methods for MSR (two kinds of approaches)

Deterministic methods

**Advantages:**
- High efficiency
- Flexibility for neutronics-thermal-hydraulic coupling
- Flexibility in kinetic calculation

**Disadvantage:**
- Relatively low accuracy in multi-heavy-isotopes condition (due to resonance)
- Limited flexibility in treating geometry

Monte-Carlo methods

**Advantages:**
- High accuracy in multi-heavy-isotopes condition
- Flexibility in treating geometry

**Disadvantage:**
- Low efficiency
- Difficulty for neutronics-thermal-hydraulic coupling
- Difficulty in kinetic calculation (both in generating kinetic parameters and time discretization)

GNU (US), SIMMER-III, DYN1D/3D (FZK)... for core analysis

MCNP+REM/Origen... for fuel cycle simulation
Serpent/RMC may be suitable for core analysis in the future
The **deterministic method** is chosen for transport/diffusion module *for its flexibility* (efficiency is not the key in current situation):

- as an independent module in steady core analysis and depletion analysis
- also as an embedded module for safety analysis

But some issues must be realized:

- Being capable of handling the **Hex-Z geometry**
  - **Easy to be achieved**
- Being accurate enough for the **multi-heavy-isotopes fuel**
  - **New methods**
Processing the ENDF/BVII by NJOY

- Evaluated Nuclear data library
- Multi-group Nuclear data library
- Resonance calculation
- Lattice transport calculation
- Lattice depletion calculation
- Homogenized XS preparation
- 3D diffusion calculation

69-groups of micro-XS for the thermal reactor & detailed information for resonance calculation (by modified the modules of NJOY)
The hyper-fine method for resonance spectrum

Over 10,000 hyper-fine groups are divided in the resonance region, but the efficiency become a new problem

Hyper-fine groups for solving slowing down equation

\[ V_i \Sigma_i (u) \phi_i (u) = \sum_{j=1}^{J} P_{ji} (u) V_j \sum_{k=1}^{K} Q_{jk} (u) \]

High accuracy and no limitation in the multi-heavy-isotopes condition, with acceptable efficiency
The collision possibility method

A numerical ‘Ray-Trace’ method based on

\[ \sum_{i,j,g} \phi_{g,i} V_i = \sum_{j=1}^{I} \left[ \sum_{g} \left( \sum_{j,g \rightarrow g} + \frac{\chi_g}{k} (v\Sigma_f)_{j,g} \right) \phi_{g,i} \right] V_j P_{ij,g} \]

\( i = 1,2,\ldots,I; \ g = 1,2,\ldots,G \)

If we can obtain the Pij, the equation can be easily solved, which depends on the geometry of lattice.
No extra difficulties if we have the reliable library and usable burn-up chain in the depletion calculation.

The homogenization method:

$$\Sigma_{x,g} = \frac{\sum_{n \in g} \sum_i \Sigma_{x,n} \phi_{n,i} V_i}{\sum_{n \in g} \sum_i \phi_{n,i} V_i}$$

Depends on the given core structure.
3D finite difference methods using rectangle mesh and tri-angular mesh
Other issues (under development)

Thermal-hydraulic calculation: single model is acceptable

Fine depletion analysis of the core: full-core micro-depletion method

Kinetic: IQS method considering the delay of precursor in the loop
Content

I • Background
II • Our activity
III • Verifying and Validation
IV • Conclusion
Verify

PWR assembly benchmark

The result with BA inside at 300K

<table>
<thead>
<tr>
<th>Reference</th>
<th>Our result</th>
<th>error/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.15773±0.00034</td>
<td>1.15668</td>
<td>0.0907</td>
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</table>

The result with control rod in at 300K

<table>
<thead>
<tr>
<th>Reference</th>
<th>Our result</th>
<th>error/%</th>
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</thead>
<tbody>
<tr>
<td>1.01057±0.00034</td>
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## BN600 benchmark from IAEA

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<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
<th>$\beta_{\text{eff}}$</th>
<th>$\beta_{\text{ef}}$</th>
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<tbody>
<tr>
<td>CEA/SA</td>
<td>1.00513</td>
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<td>0.98974</td>
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<td>3.480E-3</td>
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<td>JNC</td>
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<td>Our code</td>
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<th>HEZ</th>
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<th>AB</th>
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<tr>
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<td>CIAE</td>
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<tr>
<td>Our code</td>
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<td>48.304</td>
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</table>
## Validation

### TMSR Model

The comparison of lattice calculation in the ‘cell’ lattice 300K

<table>
<thead>
<tr>
<th></th>
<th>Keff</th>
<th>error</th>
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<tbody>
<tr>
<td>MCNP</td>
<td>1.61375</td>
<td>~</td>
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<tr>
<td>Our code</td>
<td>1.61401</td>
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Homogenization

Fuel Cell

Graphite Cell

Upper fuel zone
Main difficulty on the circular fuel zone

13 volume-weighted averaged hexagonal homogenized cell
Comparisons of $k_{eff}$

<table>
<thead>
<tr>
<th></th>
<th>$k_{eff}$</th>
<th>error</th>
</tr>
</thead>
<tbody>
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<td>MCNP</td>
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<td>~</td>
</tr>
<tr>
<td>Our code</td>
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</table>

For 300K

For different temperature

* The code could flexibly calculated the parameters of reactor core at any temperature by XS interpolation

* The references are supplied by SINAP, CAS
Reactivity coefficients

* The density is assumed to be related to the temperature by

\[
\rho = 2.263 \times (1 - 2.12 \times 10^{-4} \times (T(\degree C) - 650))
\]
Burn-up simulation (10MW U salt)

Keff

Change of U-235 fraction

Change of Pu-239 fraction
Burn-up simulation (500MW U-Th salt)

* Current model is simply magnified and the loading mass of heavy isotopes is U233-42.351kg/Th232-803.686kg

Change of U-233 fraction

Change of Th-232 fraction
The code for the **core analysis** (done), kinetic analysis and depletion analysis of TMSR is under developing.

The current work is focus on the key solver in the code: **the 3D steady neutronics solver**.

The **deterministic method** is chosen and two-step computational approach based on the homogenization theory is applied for its **flexibility** in coupling with thermal-hydraulic calculation and kinetic calculation.

The **new multi-group library** for reactor core calculation is developed. Several techniques including the **hyper-fine group method and FDM using triangular mesh are involved** to overcome the limitations due to the feature of MSR.

The code is verified by several benchmarks and validated by the TMSR model. The results prove that the current version of the code is reliable and can be used for the preliminary evaluation of TMSR.
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Thank you for your attention!

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