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Modeling and Simulation of Dispersion Particle Fuels in Monte Carlo Neutron Transport Calculation

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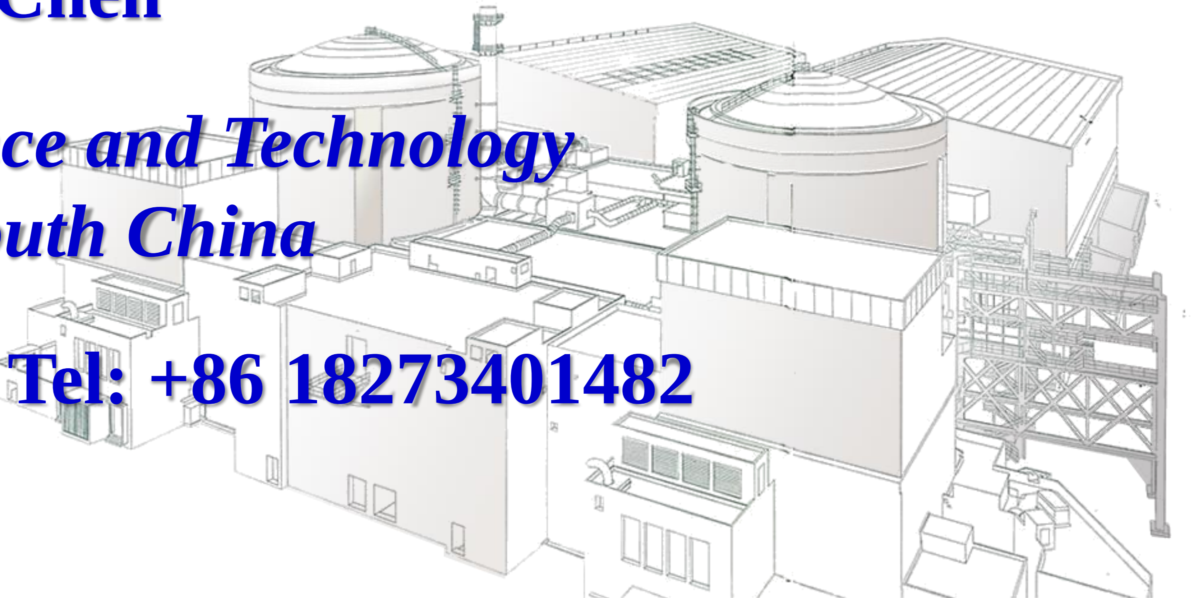
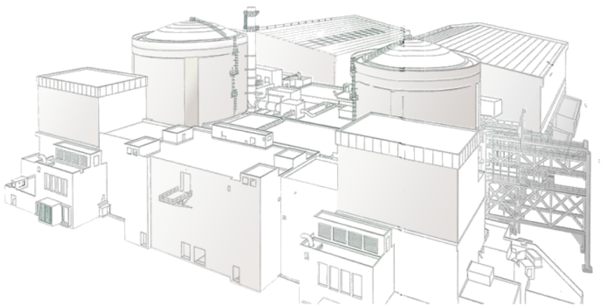


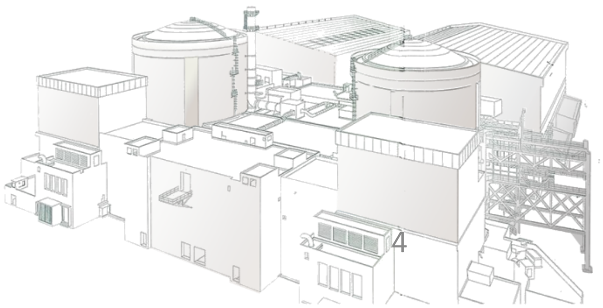
Content



I. Background

Dispersion Particle Fuel

- **Much interest lately in analyzing Dispersion Particle Fuel (DPF)**
  - Fuel kernels with several layers of coatings
  - Very high temperatures
  - Contain fission products
  - Safety aspects
- **Double heterogeneity problem**
  - Fuel kernels randomly located within fuel elements
  - Fuel elements may be "compacts" or "pebbles" (maybe random)
  - Challenging computational problem
- **Monte Carlo codes can faithfully model the DPF**
  - Full 3D geometry
  - Multiple levels of geometry modeling
  - Random geometry modeling ??



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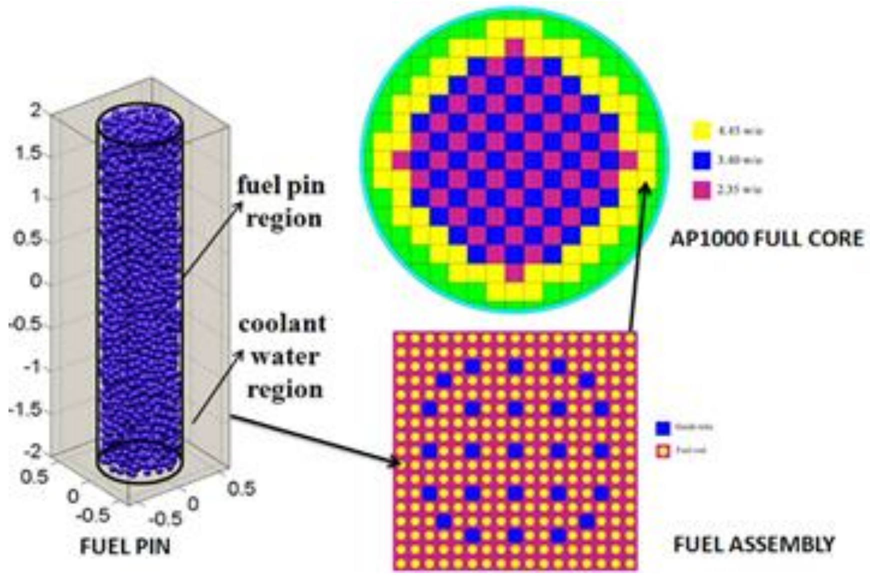
Example – HTGR

Pebble-bed reactor fuel configuration. From left to right: TRISO fuel particle, fuel pebbles, and reactor core.

Prismatic-block gas-cooled reactor fuel configuration. From left to right:TRISO fuel particle, fuel compact, fuel block, and reactor core.

Example – FCM-type PWR



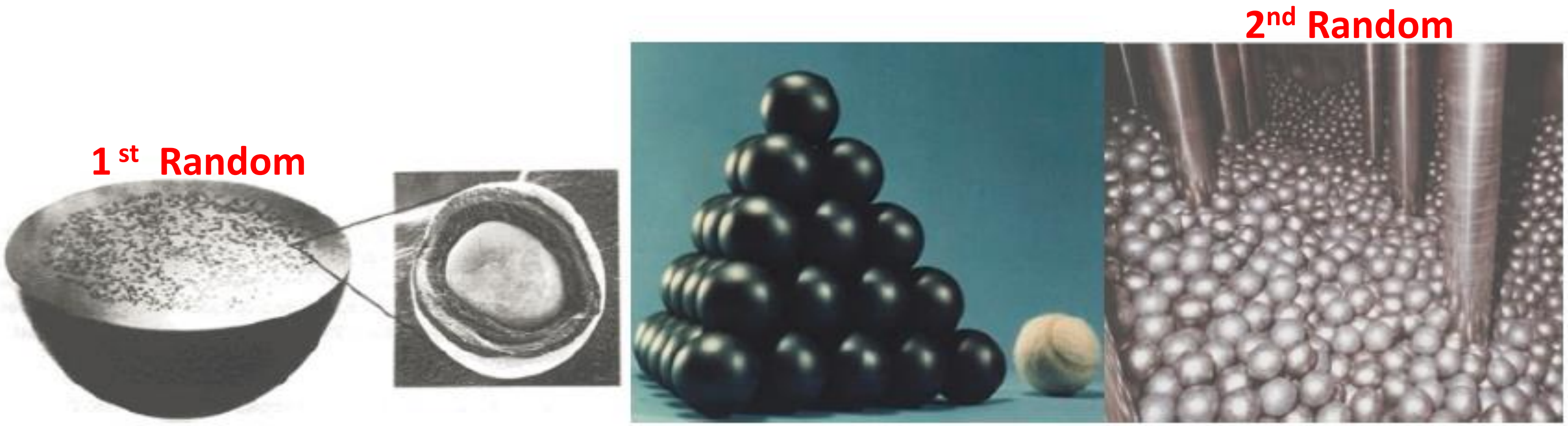
FCM fueled LWR configuration at different dimensional levels: from TRISO fuel particle to LWR core assembly

Challenges

- **Double heterogeneity problem**

– Fuel kernels randomly located within fuel elements

– Fuel elements may be "compacts" or "pebbles" (maybe random)

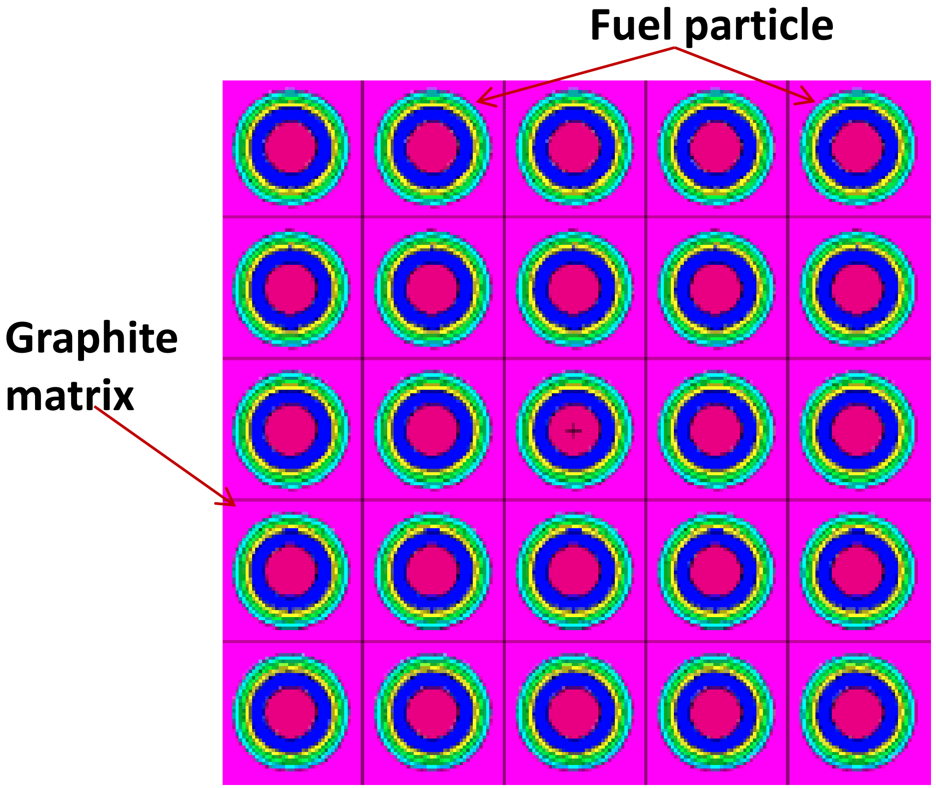


Pebble-bed reactor fuel configuration. From left to right: TRISO fuel particle, fuel pebbles, and reactor core.

How to model the RANDOM distribution of DPFs in Monte Carlo simulation ?

II. Methods and Implementations

Lattice-based modeling method



Conventional lattice modeling for DPFs in Monte Carlo simulation

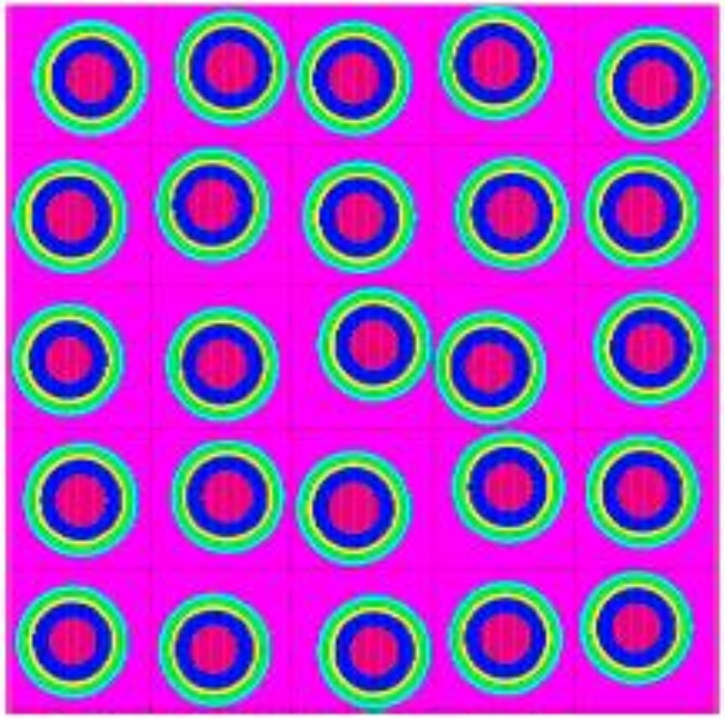
- Lattice model is one of the most commonly used methods for DPFs modeling.

- A series of regularly distributed lattice grids are constructed, and each fuel particle is placed at the center of the lattice grid. Each lattice grid contains only one fuel particle.

- The biggest drawback of the method is difficult to maintain the required fuel volume packing fraction (usually less than 0.524). It is difficult to be applied in engineering application.

- It can not consider the random distribution of fuel particles in the graphite matrix, so the effective multiplication factor in the assembly calculation results in an error 0.1%~0.2%, and greater errors will be produced for the whole core calculations.

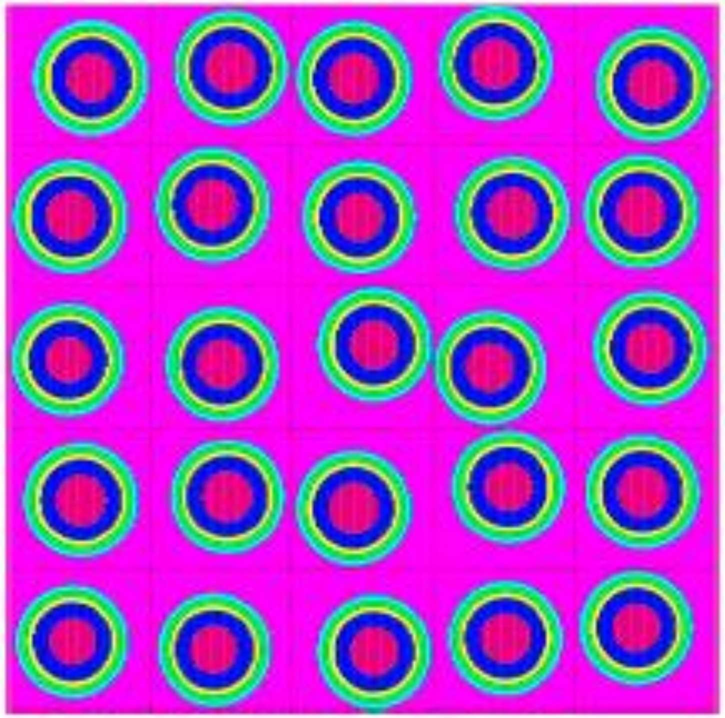
Sub-Fine Lattice (SFL) method



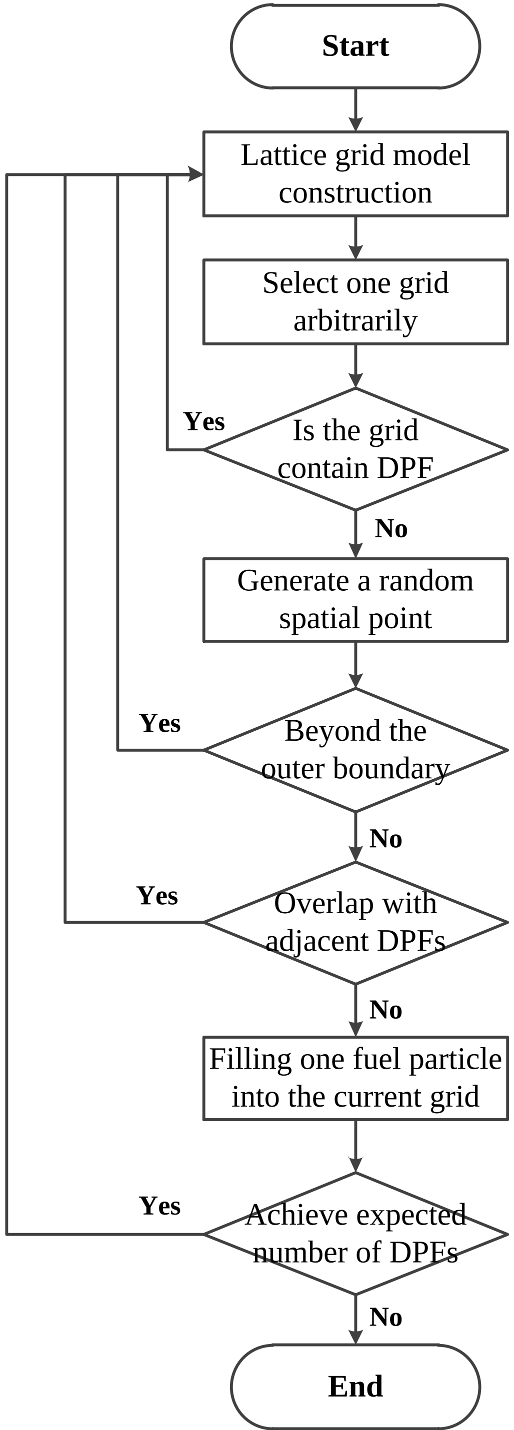
Sub-Fine Lattice Modeling for DPFs in Monte Carlo simulation

- The Sub-Fine Lattice method is a random distribution model, which is further developed from the conventional lattice-based modeling method.
- Compared with the conventional lattice model, the sub-fine lattice modeling method also uses the regular distributed lattice grid to place the fuel particles, but the central points of the fuel particles are randomly distributed in the lattice grids.
- The size of the lattice grid is not needed to be strictly specified.
- Therefore, the sub-fine lattice model is a stochastic model which takes into account the stochastic distribution of fuel particles in the graphite matrix.

Sub-Fine Lattice (SFL) method



Sub-Fine Lattice Modeling for DPFs in Monte Carlo simulation



The basic principle and implementation procedure of the SFL method.

Method implementations

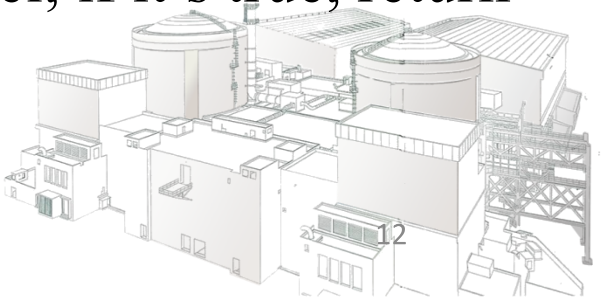
(1) A three-dimensional lattice grid model with regular distribution is established;

(2) A lattice grid is selected randomly, and then determining whether the selected grid is filled with fuel particle or not;

(3) If the selected lattice grid has been filled with fuel particles, return to step (2); otherwise, enter into step (4);

(4) In the selected lattice grid, a spatial point will be generated randomly using the sampled pseudo random number, and the center of the fuel particle will be placed at that point;

(5) Check whether the fuel particle beyond the outer boundary of the model; if it’s true, return to step (2), otherwise go forward into step (6);

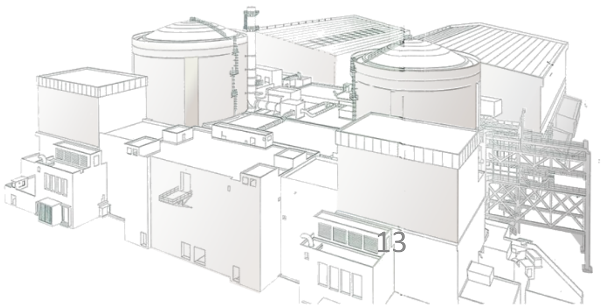


Method implementations

(6) Check whether the fuel particle in the current lattice grid overlap with the fuel particles located in the adjacent lattice grids; if it's true, return to step (2), otherwise enter into step (7);

(7) A fuel particle is placed at the generated spatial point in the current selected lattice grid;

(8) Determine whether the fuel particles filled in the model achieve the expected number, or whether the volume packing fraction of the fuel particles reaches the expected value; if not, return to step (2); otherwise, the modeling will be established.



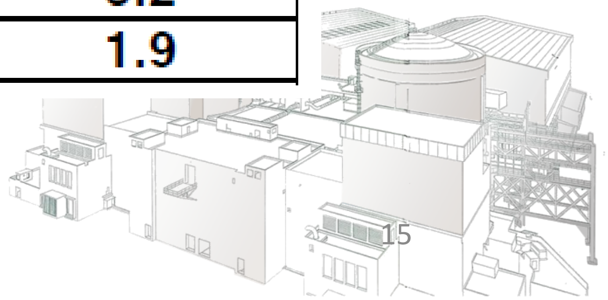
III. Numerical Results and Analysis

Benchmark specification

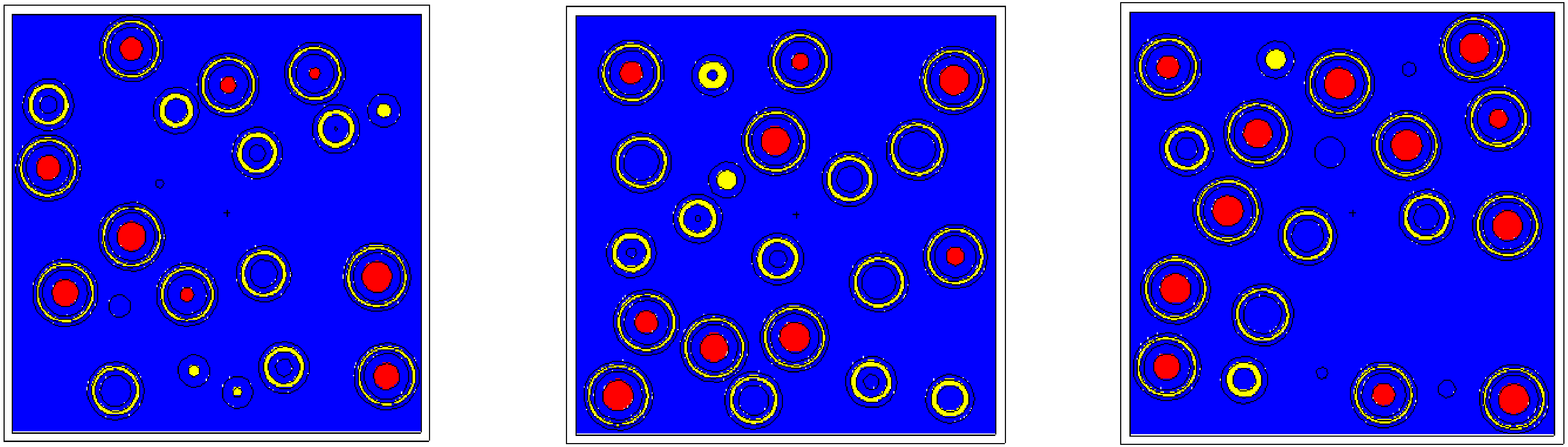
- A graphite matrix cubic model with a side length of 0.4754 cm was defined, and 100 TRISO coated fuel particles were randomly filled in the model based on the Sub-Fine Lattice (SFL) method.
- The specific materials, dimensions and specific geometries of the TRISO fuel particles used in the model are taken from the NGNP high temperature gas reactor design.
- The infinite multiplication factor (k_∞) of the model was calculated using MCNP code.

TRISO Fuel Kernel Geometry and Composition

Region #	Name	Outer radius (μ)	Composition	Density (g/cc)
1	Uranium oxycarbide	175	UCO ($UC^{.5}O^{1.5}$)	10.5
2	Porous carbon buffer	275	C	1.0
3	Inner pyrolytic carbon	315	C	1.9
4	Silicon carbide	350	SiC	3.2
5	Outer pyrolytic carbon	390	C	1.9



Numerical Verification



The X-Y/Y-Z/X-Z cross-sectional views of the cubic model

Table 1. Sub-Fine Lattice (SFL) model numerical verification

Modeling method	k_∞	Statistical error(σ)
SFL method	1.29265	0.00087
RSA method	1.29058	0.00095

Impacts of SFL grid sizes on efficiency

Table 2. Modeling efficiency with SFL grid size of $2R/\sqrt{3}$

Number of fuel particles	Modeling time (s)
10	0.101
45	0.589
75	1.741
100	7.908

Table 3. Modeling efficiency with SFL grid size of R

Number of fuel particles	Modeling time (s)
10	0.097
45	0.568
75	1.507
100	7.250

Table 4. Modeling efficiency with SFL grid size of $2R/\sqrt{5}$

Number of fuel particles	Modeling time (s)
10	0.244
45	1.342
75	4.695
100	25.540

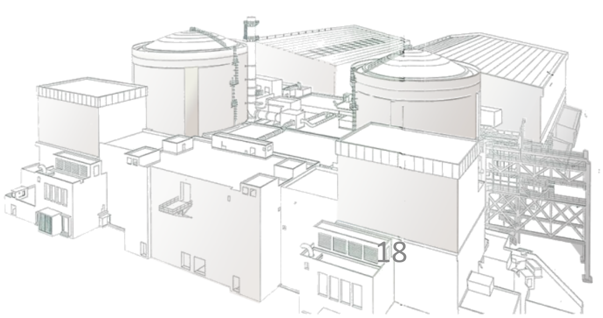
The testing is performed on a 2.2 GHz single processor Intel Core i5-5200 CPU with 8.0 GB RAM.

Impacts of SFL grid sizes on accuracy

- As the lattice grid size decreases, the number of grids that need to be overlapping checked during modeling will increase and then the modeling speed will become slower.
- Theoretically, when the lattice grid size tends to be zero, the number of grid need to be overlapping checked will also tend to be infinity. Under this situation, the sub-fine lattice model has actually been transformed into the RSA model.
- Thus, as the lattice grid size decreases, the sub-fine lattice model will tend to be the RSA model. When the lattice grid size is equal to zero, actually, the sub-fine lattice model has become RSA model.

Table 5. Impacts of different grid sizes on calculation accuracy

Grid size	k_∞	Statistical error (σ)
$2R/\sqrt{3}$	1.29265	0.00087
R	1.29134	0.00087
$2R/\sqrt{5}$	1.29032	0.00091
RSA	1.29058	0.00095 (reference)



Discussions and analysis

- With the lattice grid sizes decreasing, the sub-fine lattice model will tend to be the RSA model, which will increase the randomness of the sub-fine lattice model.
- Meanwhile, the decreasing in lattice grid sizes will lead to a rapid increase in modeling time, which makes the sub-fine lattice model lose its greatest advantage on modeling efficiency.
- When modeling efficiency is primarily considered, there is need to select a larger lattice grid size for modeling. If the calculation accuracy is primarily considered, the grid needs to be chosen with smaller sizes.
- So the randomness of the sub-fine lattice model with a grid size of R is larger than that of the model modeled with a grid size of $2R/\sqrt{3}$, and the modeling speed with a grid size of R is faster than that of the model with a grid size of $2R/\sqrt{5}$.
- To balance the modeling efficiency and calculation accuracy, it is recommended to use the grid size of R as the optimal grid size to perform the DPF fuels modeling.

Conclusions

- The basic principle and implementation scheme of SFL method for stochastically modeling the dispersion particle fuels were presented.
- The modeling efficiency and calculation accuracy of the SFL method were tested and verified using the TRISO-type DPF models.
- The numerical results show that the calculation results of the SFL model are in good agreement with the reference results, which demonstrates the effectiveness and correctness of the modeling method.
- The lattice grid size used in the sub-fine lattice model will have a great influence on the modeling efficiency and the calculation accuracy.
- To balance the efficiency and accuracy, it is recommended to use a grid size of R as the optimal size in DPF modeling and simulation.

Thanks for your Attention.