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Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

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Processing and Utilization of Nuclear Reaction Data for Advanced Gas Cooled Reactor (AGCR) Applications

Lecture 1 – Physics and Theory

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IAEA/ICTP Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

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OUTLINE

- Introduction to AGCRs
- Physics of AGCRs
- Evaluated nuclear data files, data retrieval and processing
  - Resonance-self shielding treatment
  - Resonance scattering modeling
  - Energy group structures and their optimization
- Conclusions

INTRODUCTION TO AGCRs

- High Temperature Gas Reactor (HTGR) concept originated in the late 1950s
- Developed and tested in a number of critical experiments (for example in the KAHTER facility in Germany)
- Test reactors, like the 20 MW DRAGON reactor in England, the 115 MW Peach Bottom reactor in the USA, and the 46 MW AVR pebble bed reactor in Germany
- Later, two larger prototype reactors were built: a prismatic block type HTR in Fort St. Vrain (Colorado, USA) of 842 MW and the THTR-300 in Uentrop-Schmehausen (Germany), a pebble-bed type HTR of 750 MW

INTRODUCTION TO AGCRs

- ACACIA, a 40MW pebble-bed reactor design project in the Netherlands
- The HTR-10 in China is a small HTR (10 MW) and is the only pebble-bed reactor in operation today
- The first criticality of the Japanese HTTR (30 MW) (of prismatic core) was attained in November 1998.
- The US Department of Energy has identified Very High Temperature Gas Cooled Reactor System (VHTR) as a candidate for both hydrogen production and electricity generation.
- In South Africa, advanced design work has been performed of a modular HTR the PBMR.

INTRODUCTION TO AGCRs

Pebble Bed Reactor Experience

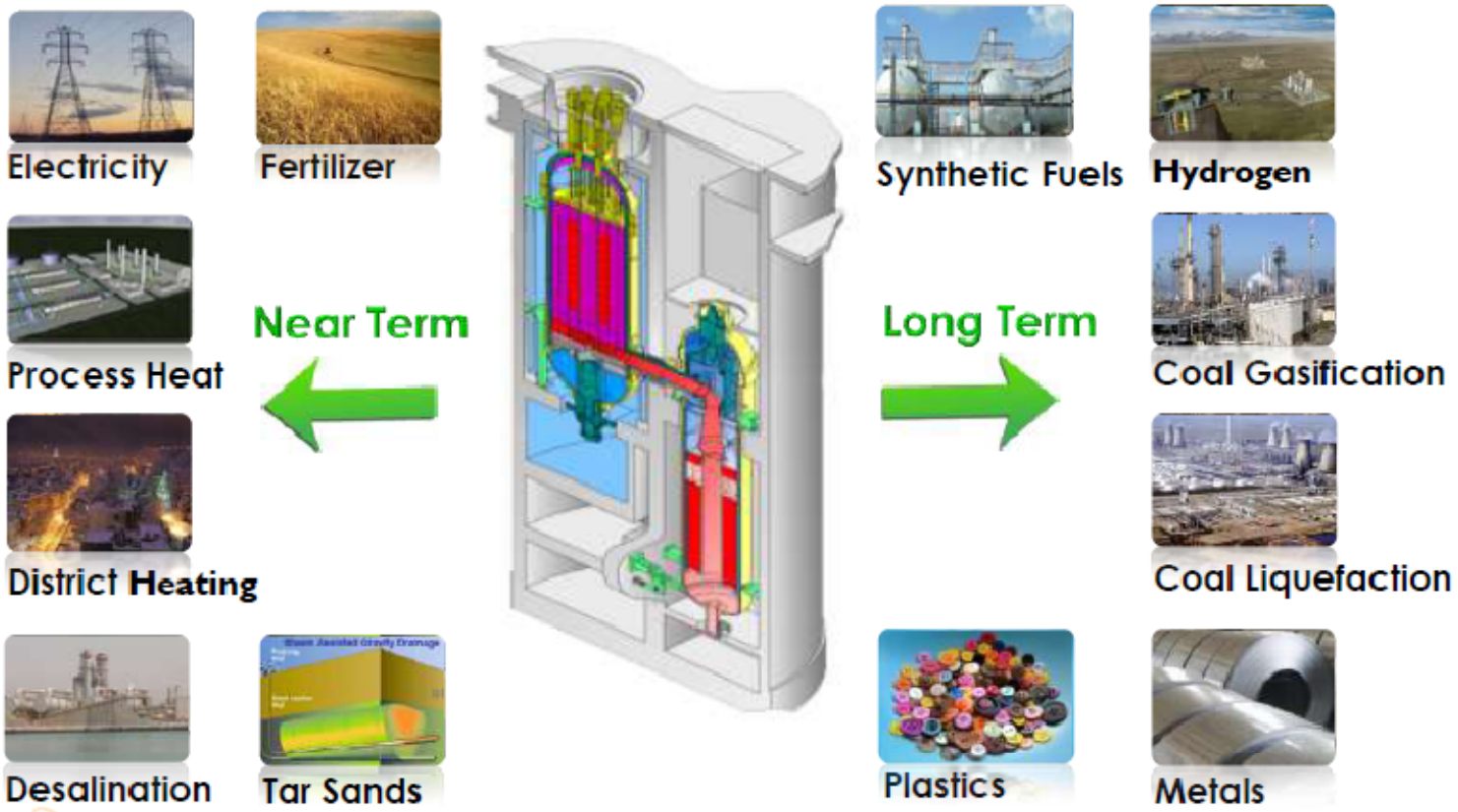
Major Projects	Power (MWt)	Status
AVR (Germany)	50	Being Decommissioned
THTR 300 (Germany)	750	Decommissioned
HTR 500 (Germany)	1390	Prel Design/Lic Review Archived
HTR 100 (Germany)	250	Prel Design/Lic Review Archived
HTR Modul (US, Germany)	200	Prel Design/Lic Review Archived – Safety Concept License Approved
DPP 400 (South Africa)	400	Prel Design/Lic Review Archived – Major Components Canceled
HTR-10 (China)	10	Operating
PM-250 (China)	250	Construction Underway
PBMR-CG (NGNP)	250	Conceptual Design Underway

Introduction to AGCRs

- **Interest in the HTGR is the result of its enhanced safety characteristics, thus:**
  - **The use of coated particles which retains fission products up to a fuel temperature of 1600^0C, as confirmed by experiments**
  - **Use of graphite as both moderator for neutrons and as construction material**
  - **The use of helium as coolant**
  - **The low power density (2 to 6 MW/ m^3, compared to at least 50 MW/m^3 for a LWR)**
  - **A continuous fuel supply in case the core consists of spherical fuel elements, limiting the excess reactivity in the core to a minimum.**

INTRODUCTION TO AGCRs

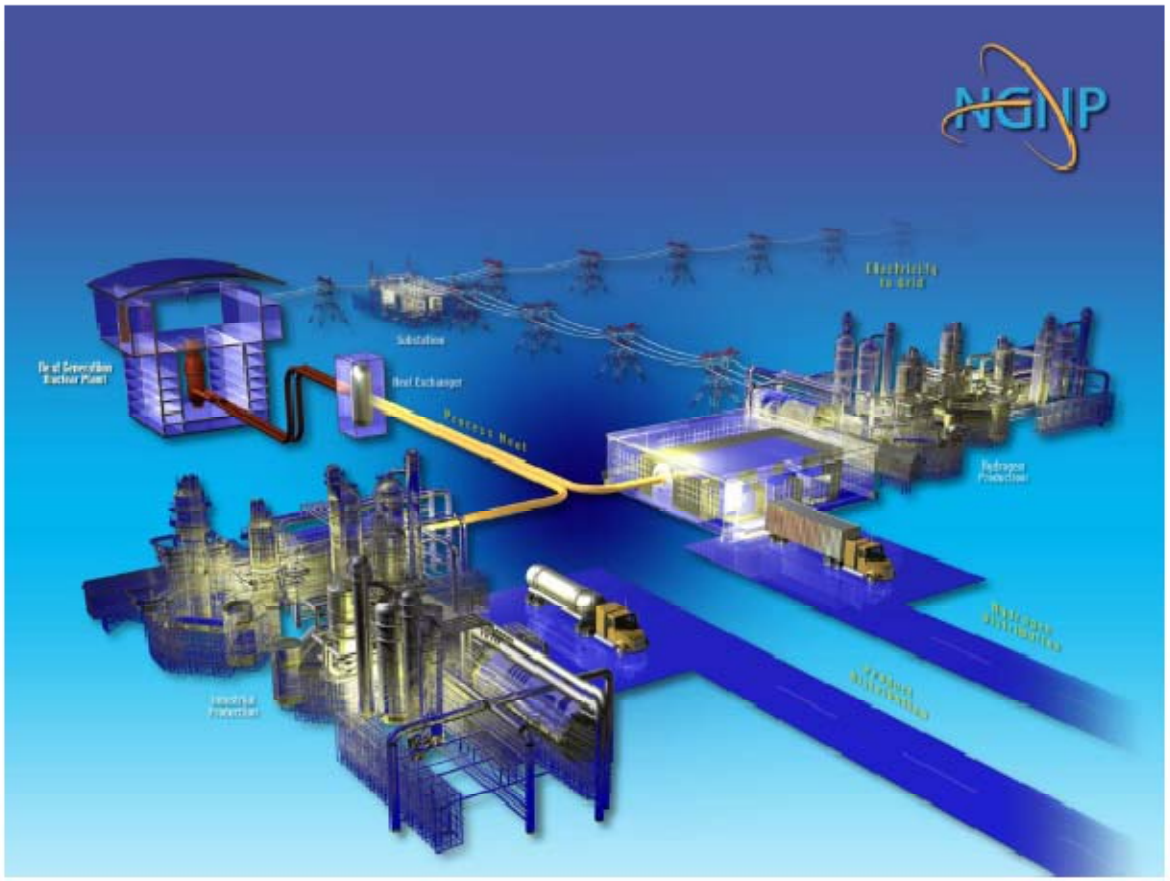
Gas Reactors Are Central to Future Energy Needs



INTRODUCTION TO AGCRs

- **Next Generation Nuclear Plant (NGNP): Enables Nuclear Energy to Enter Other Markets Beyond Electricity**

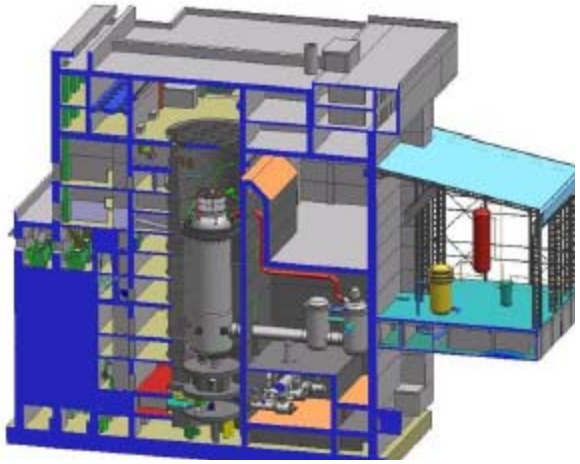
NGNP: Process Heat, Hydrogen, and Electricity



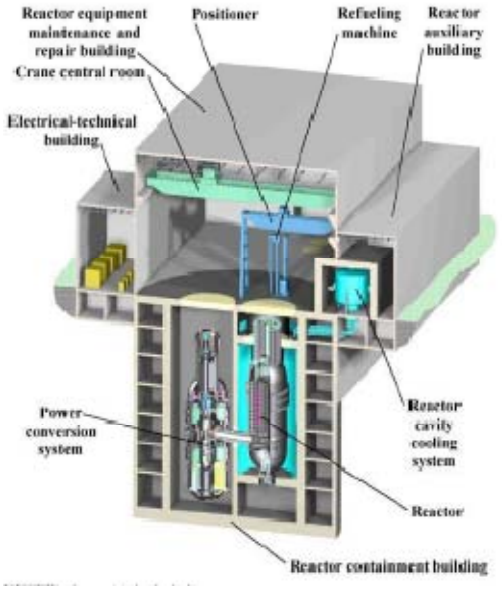
INTRODUCTION TO AGCRs

- **Two pre-conceptual designs for NGNP:**

Pebble-Bed

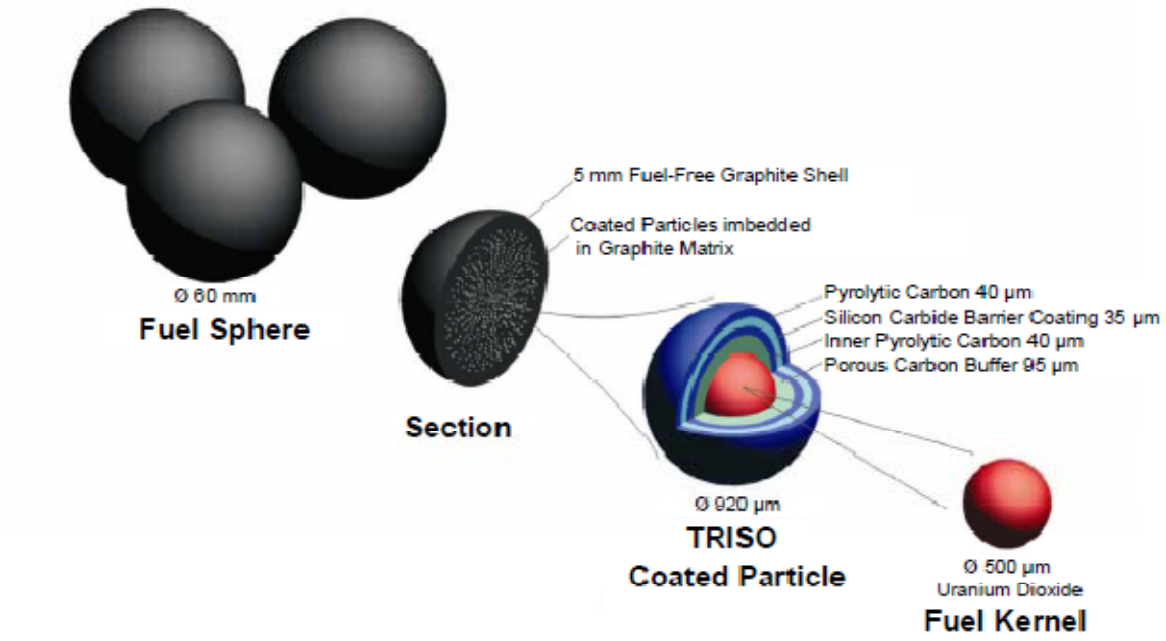


Prismatic

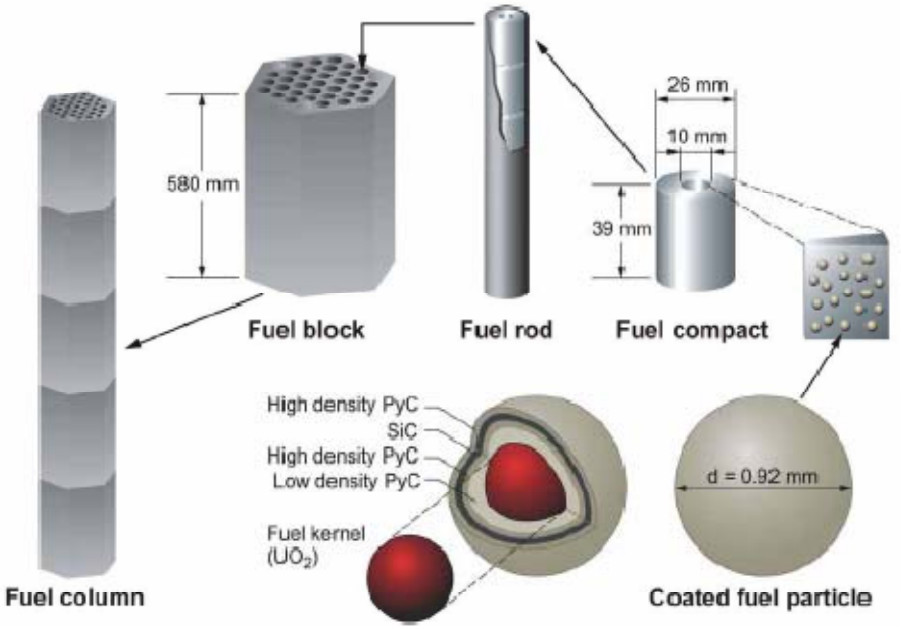


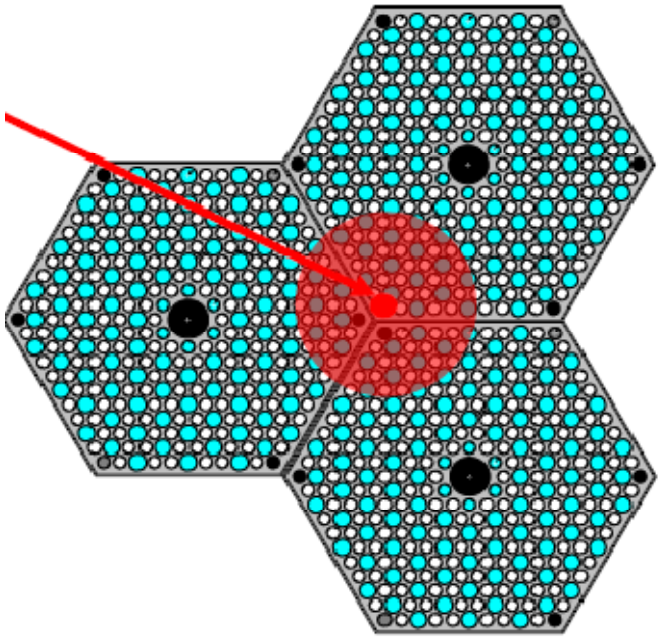
INTRODUCTION TO AGCRs

Fuel Pebble Design – Proven Fuel Performance



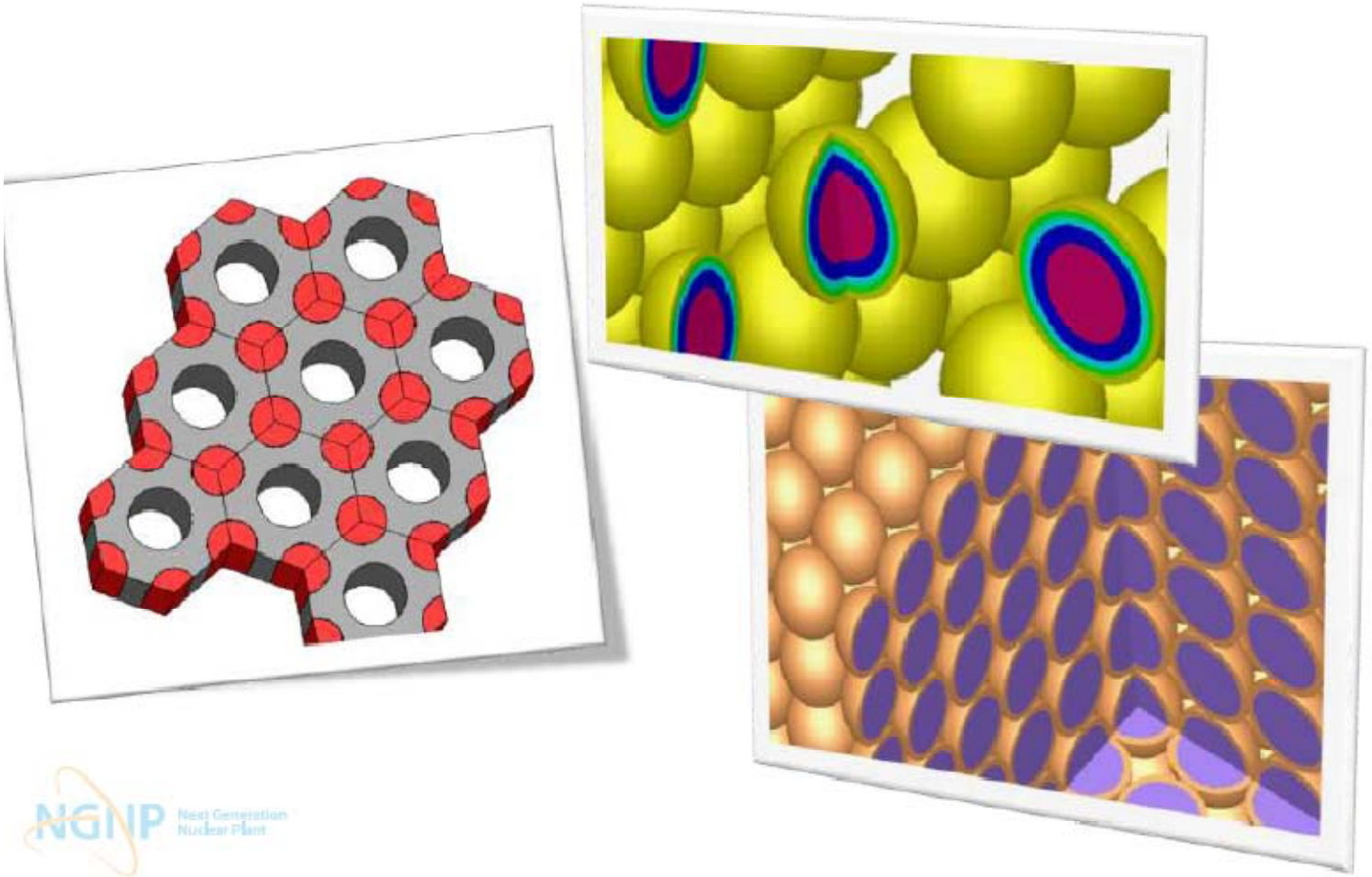
INTRODUCTION TO AGCRs





INTRODUCTION TO AGCRs

Infinite Lattice Configurations



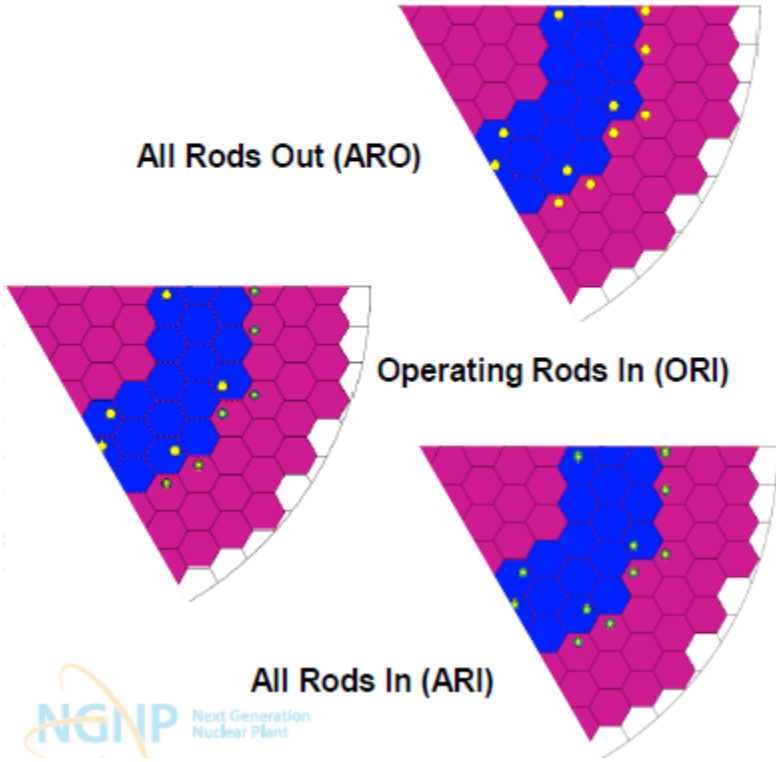
NGNP Next Generation Nuclear Plant

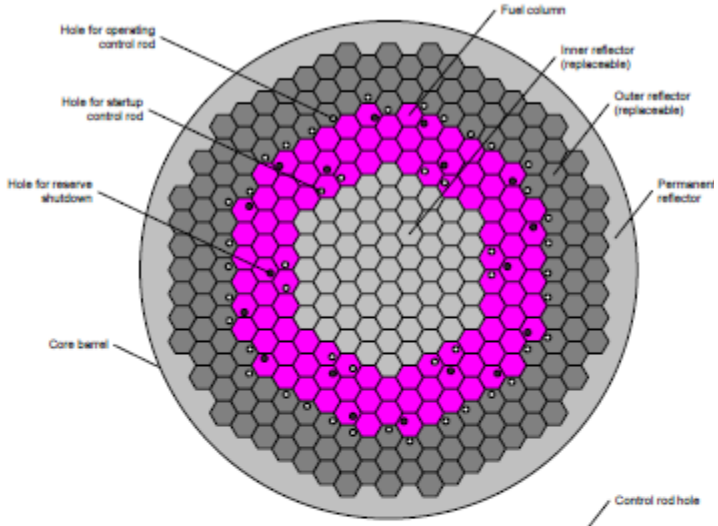
INTRODUCTION TO AGCRs

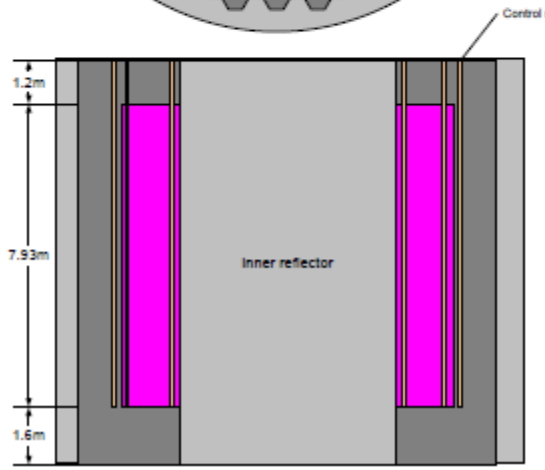
NGNP/VHTR Benchmark Problems

- **Two sets of benchmark cores**

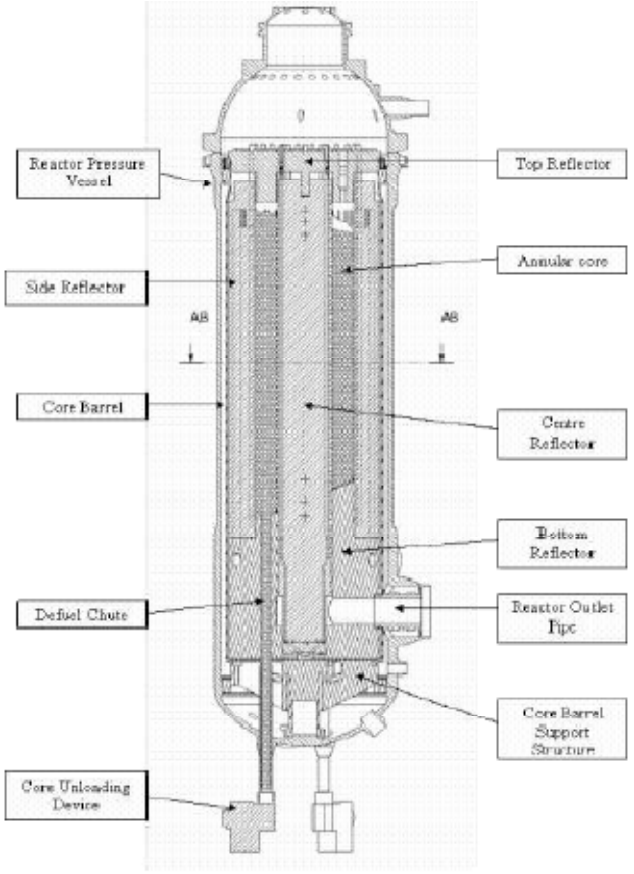
  14 w/o and 10 w/o U-235 fuel compact (25% packing fraction)

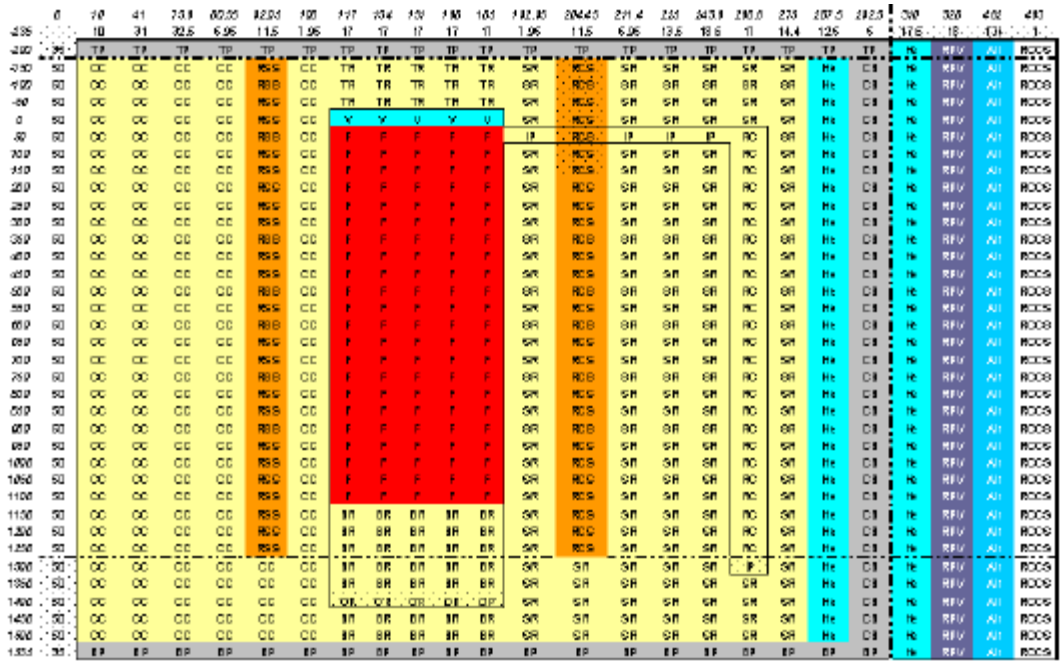






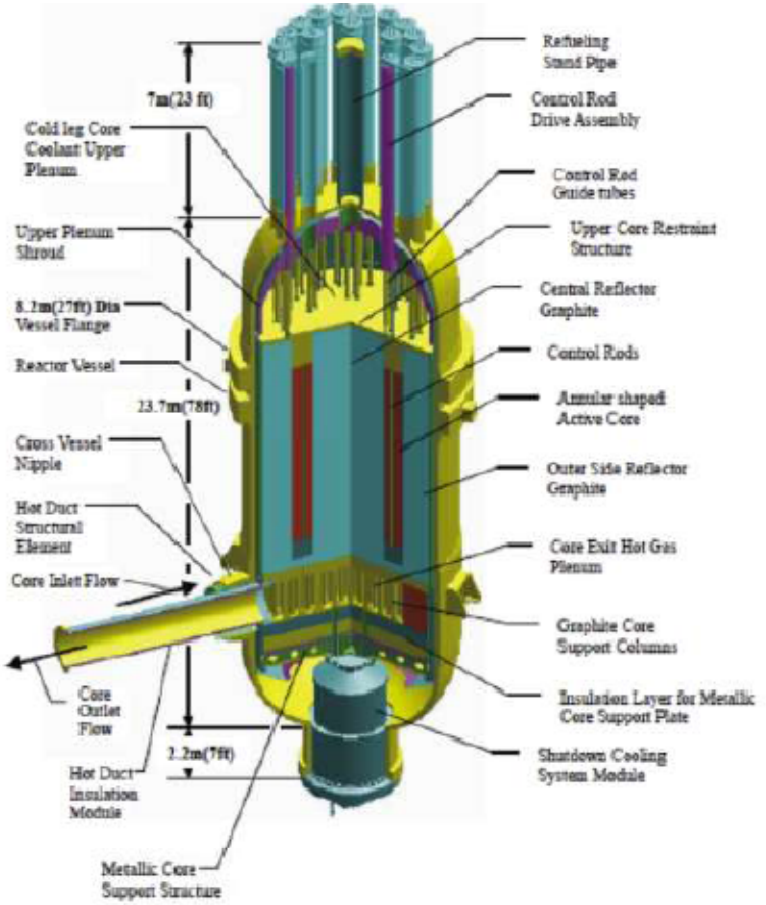
INTRODUCTION TO AGCRs





PHYSICS OF AGCRs

- Physics of high temperature reactors is different from that of other types of reactors
- Anticipated operating and accident scenarios feature safety-relevant fluid behavior not captured with existing tools
- Analytical tools used by designers employ approximate methods that have not changed in decades
- Advanced analytical tools have not been validated for licensing purposes



PHYSICS OF AGCRs

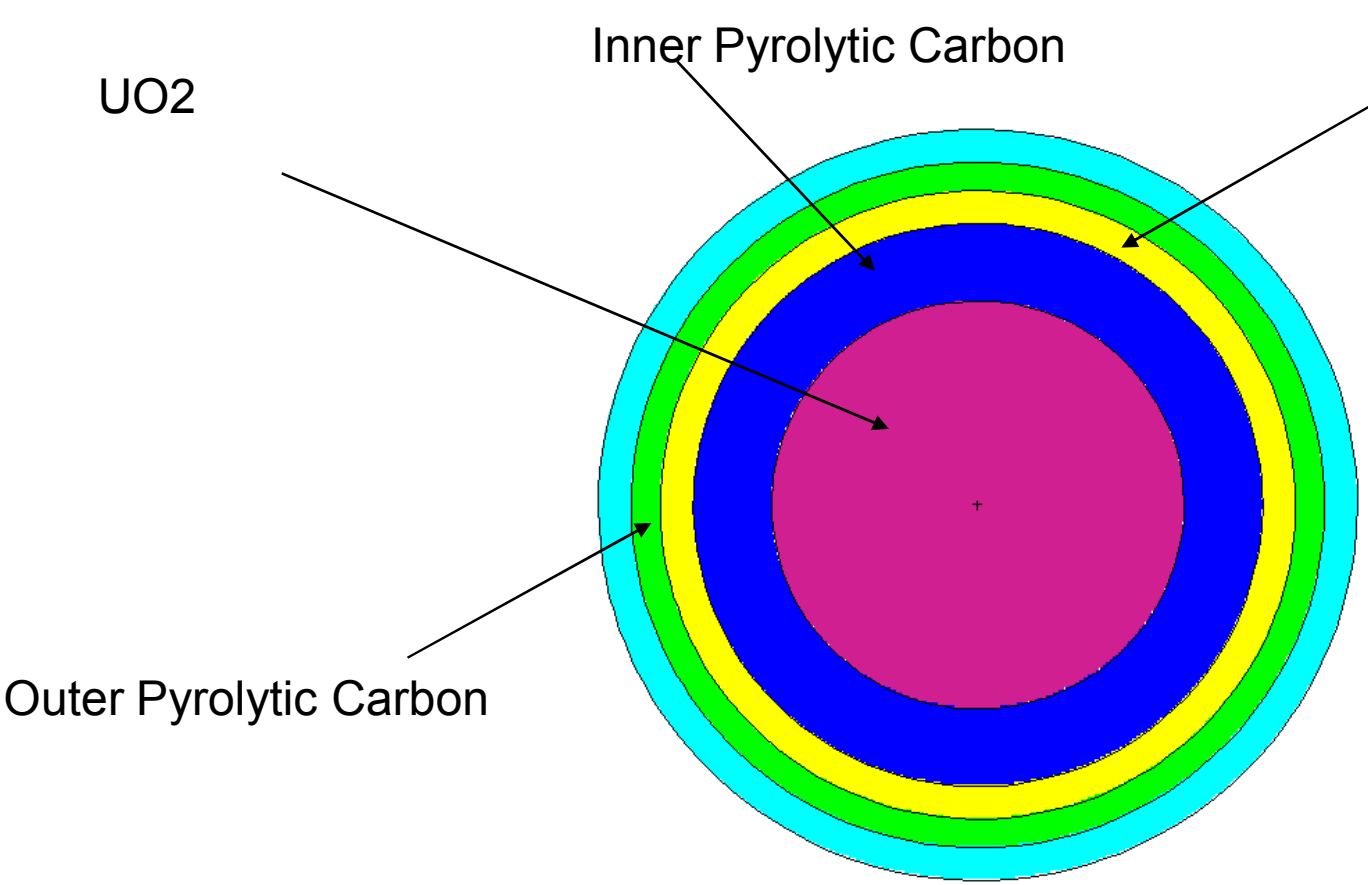
- Nominal reactor control is achieved with control rods inserted into the reflector
- Load following is also achievable through manipulation of the helium inventory of the primary loop
- Use of graphite as moderator has both advantages and disadvantages
  - low absorption cross-section = higher moderating ratio but crystalline properties = a need for detailed treatment of the scattering law in physics calculations
  - low parasitic absorption rate in the overall core and reflector allows = high fuel burnup at low fuel cost but requires a higher total heavy metal loading.

PHYSICS OF AGCRs

- Higher moderating ratio (moderator atom per fuel atom) = more neutron absorptions by the fuel in the thermal energy range (85% vs. 70% in a PWR).
- Calculational methods for HTGRs places greater importance of detailed spectrum calculations (it is necessary to take a large number of energy groups)
- These designs are susceptible to transport effects due to control rod positioning in the side reflectors and the presence of the cavity at the top of the pebble-bed, where diffusion theory breaks down

DOUBLE HETEROGENEITY

Heterogeneity in the fuel kernel



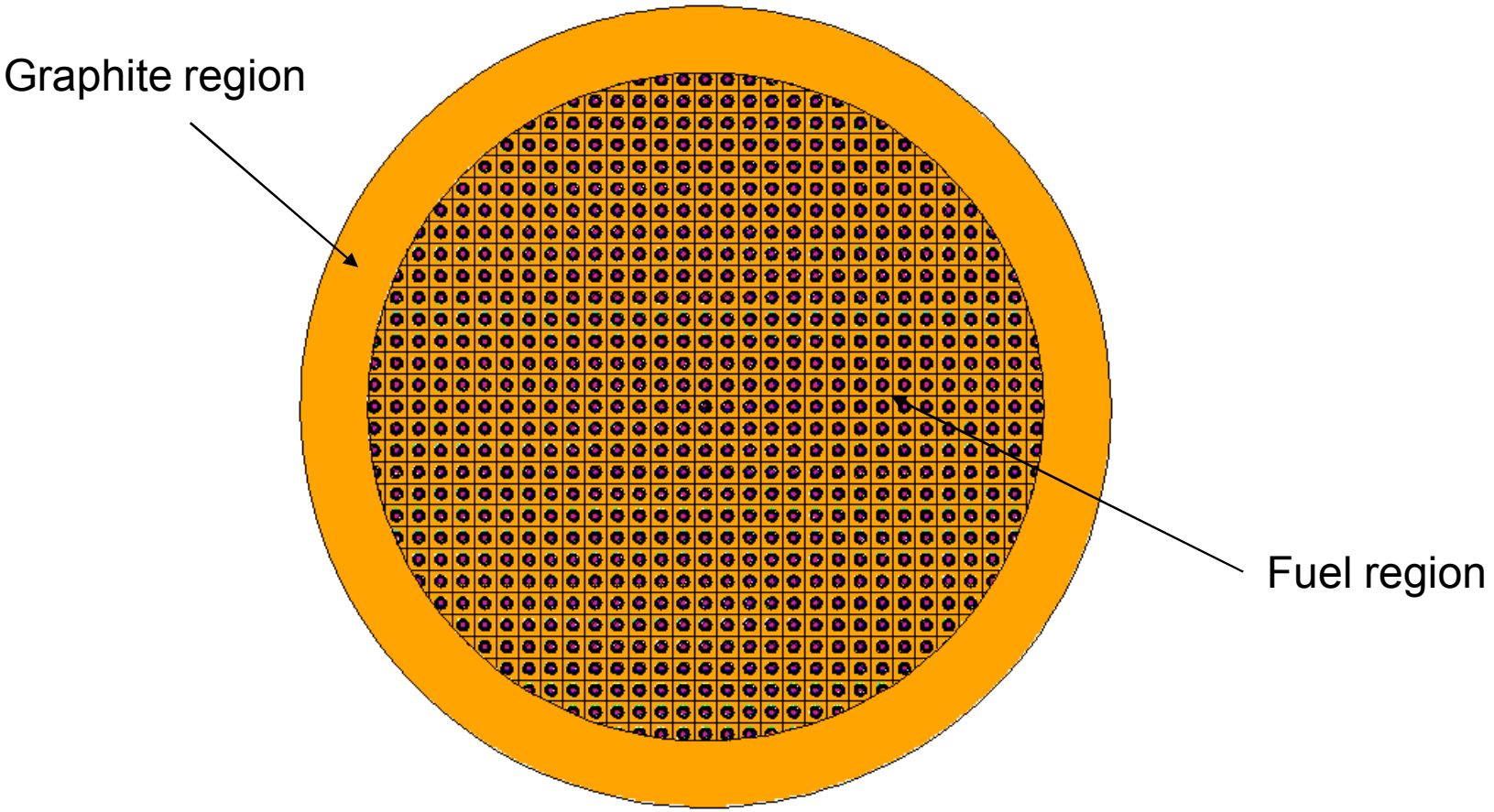
Double heterogeneity is encountered on:

a) microscopic level (kernel) and

b) macroscopic level (fuel pebble)

DOUBLE HETOROGENEITY

Heterogeneity in the pebble



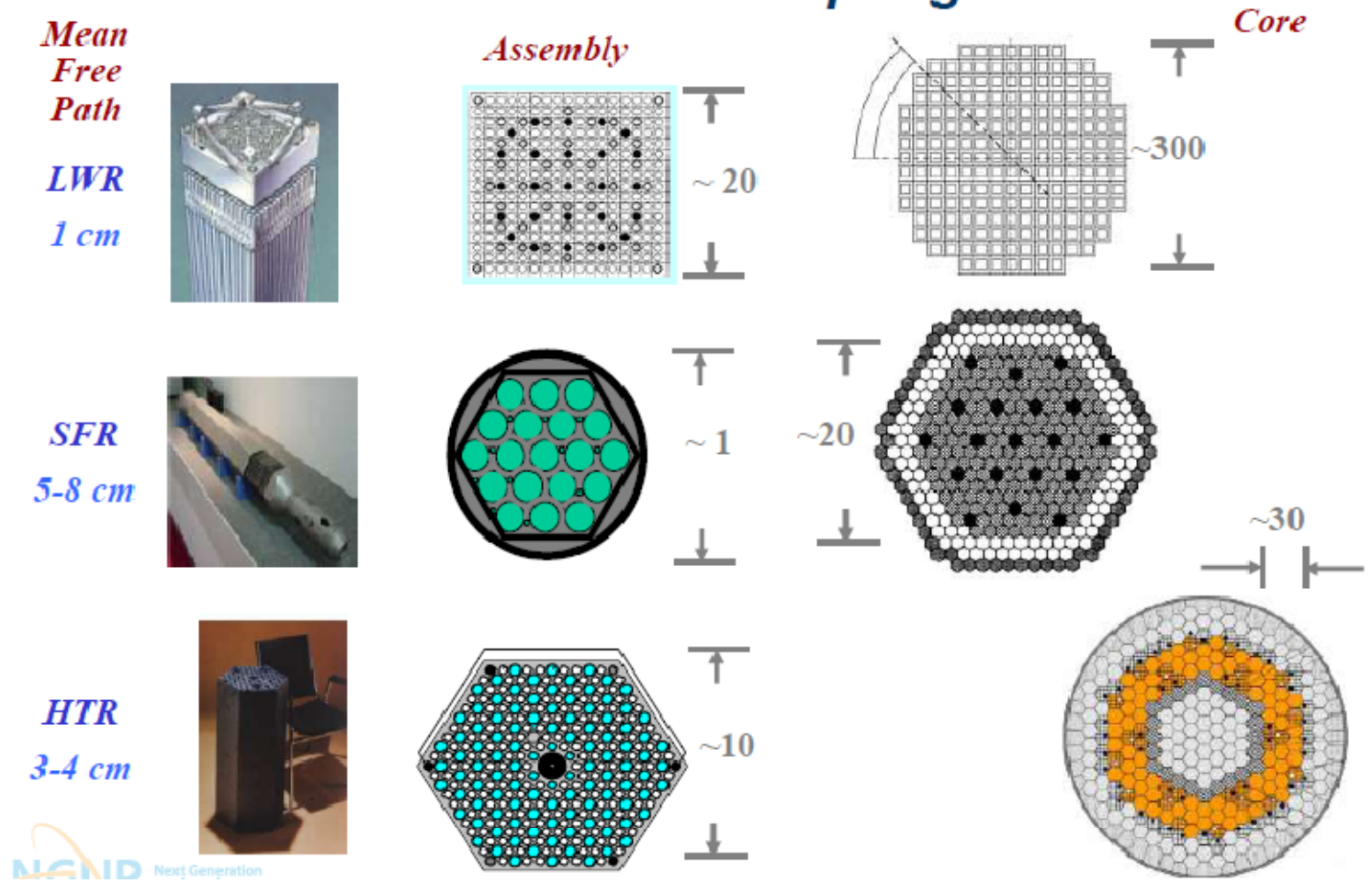
Research Focus – Systematic Error Control in Homogenization and Energy Condensation

- **Objective**: Capture the physics of HTR fuel (multiple heterogeneity, graphite and heavy metal scattering, resonance effects, spectral leakage) to improve the fidelity of core simulations and to bound the uncertainty in key safety parameters due to physics data, approximations, and assumptions
  - Generate cross sections that yield accurate results in nodal diffusion and depletion calculations
  - Parameterize cross sections to support fast but accurate transient calculations (in both system and multiphysics analyses)

- **Acceptance Criteria**: Nuclear Energy Agency (NEA) Fuel and Depletion Benchmarks, Critical Experiments, Computational References (Monte Carlo, etc.)

PHYSICS OF AGCRs

Neutronic Resolution and Coupling



Effective Microscopic Cross Sections:

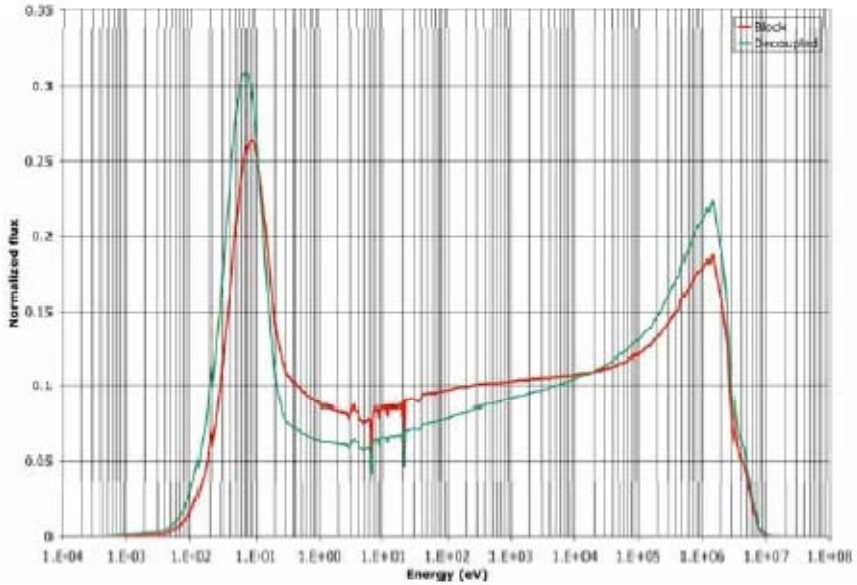
$$\sigma_g = \frac{\int_g \sigma\ E\ \varphi\ E\ dE}{\int_g \varphi\ E\ dE}$$

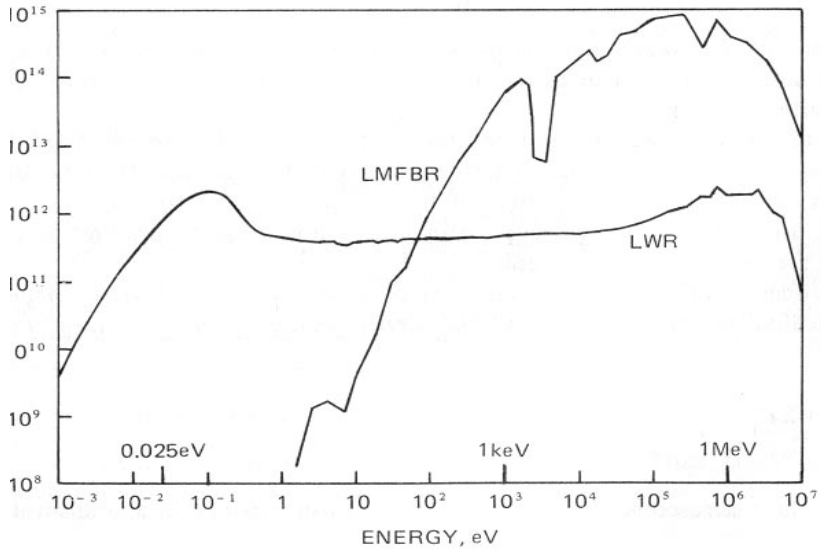
$\varphi\ E$

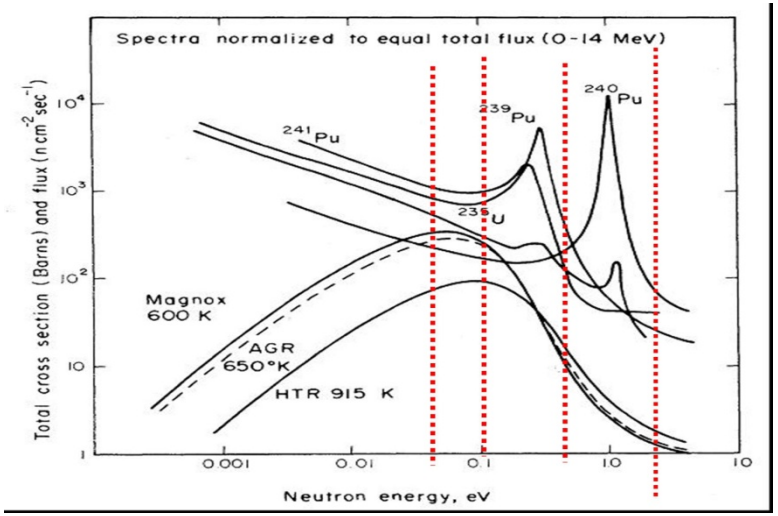
- Depends on local composition
- Depends on in-leakage from neighboring regions (inter-penetration of spectra): challenge in optically thin assemblies and cores; multiple levels of heterogeneity
- Depends on additional perturbation from transport effects in and near strong absorbers and all types of interfaces

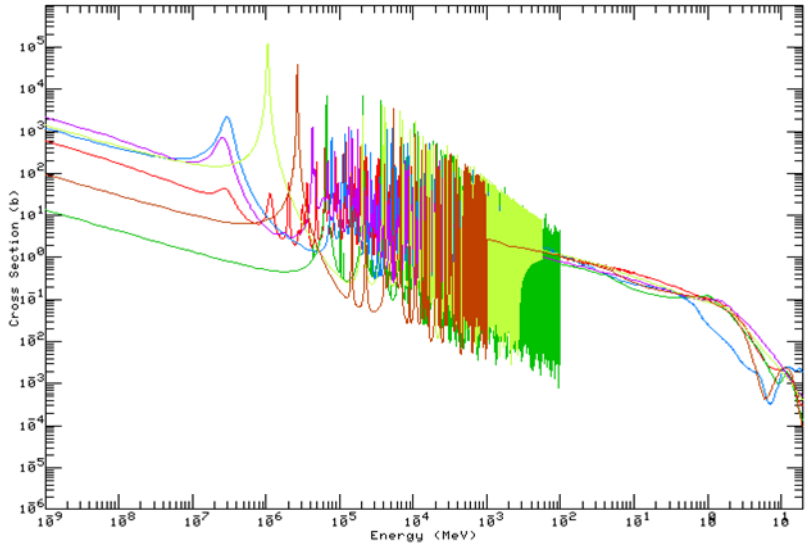
$\phi\ (\ E\ )$

PHYSICS OF AGCRs

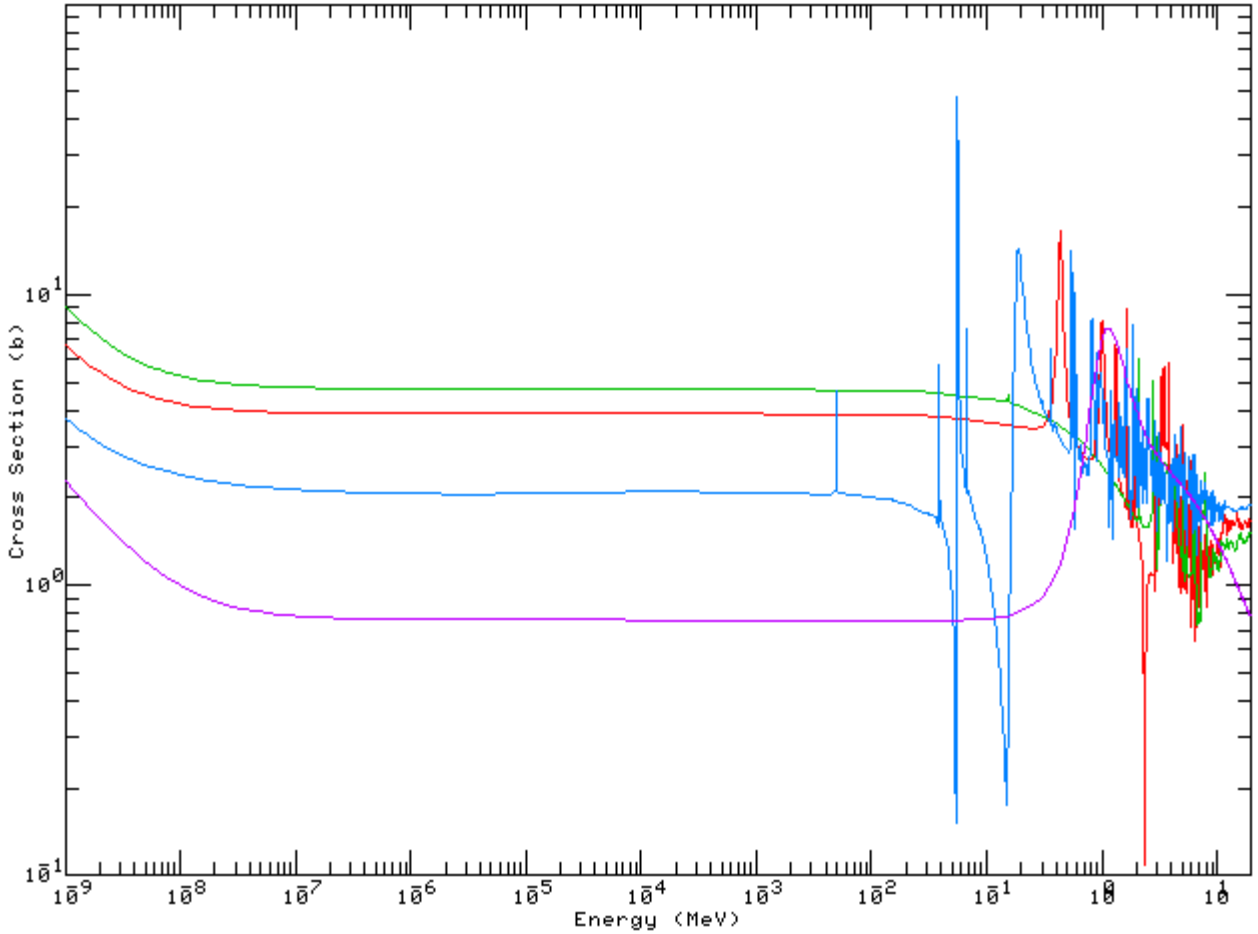








PHYSICS OF AGCRs



O-16 T=300 K from ENDF/B-6.0 mat 825 - red

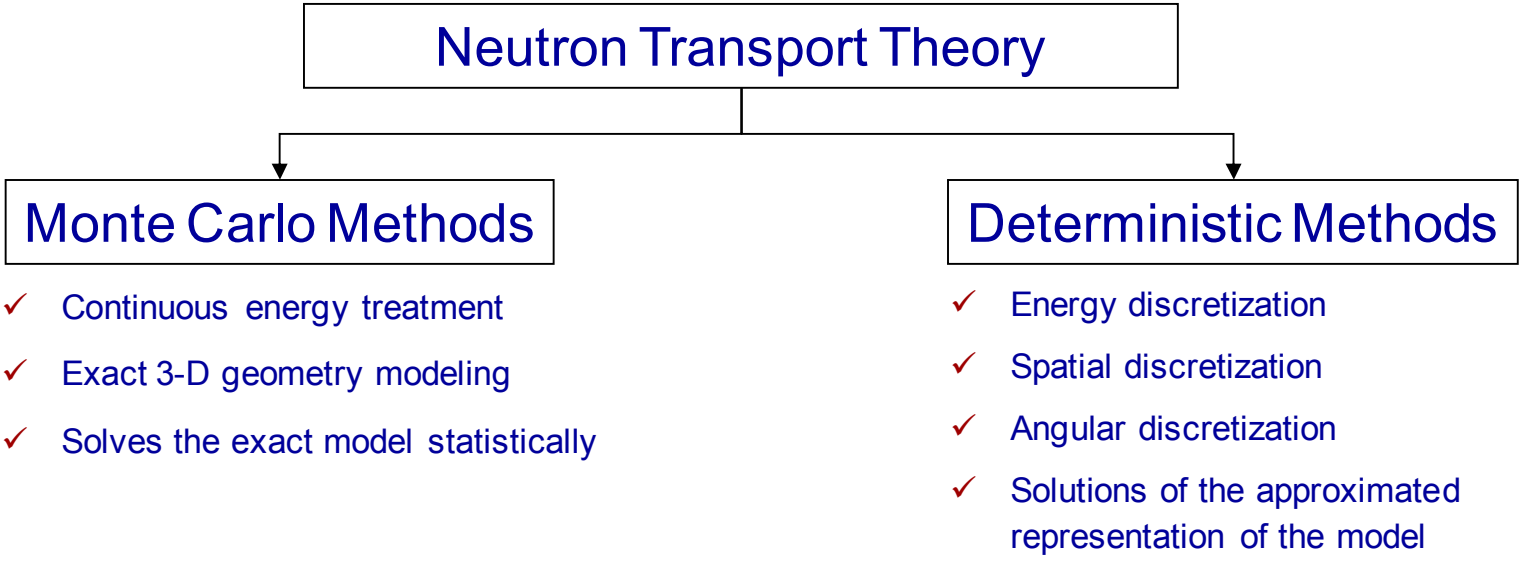
C-nat. T=300 K from ENDF/B-6.1 mat 600 - green

Si-nat. T=300 K from ENDF/B-6.0 mat1400 - blue

He-4 T=300 K from ENDF/B-6.0 mat 228 - purple

DATA PROCESSING

- ✓ **Two classes of computational methods to solve neutron transport equation: deterministic and Monte Carlo**
- ✓ **The energy discretization procedure is common to all deterministic computational methods: the multi-energy-group approximation**



DATA PROCESSING

- ✓ In the United States, the national responsibility for all information about nuclear cross sections is the National Cross Section Center (NCSC) at the Brookhaven National Laboratory (BNL) in Upton, New York.
- ✓ Cross-section data obtained either by calculation, or experiment, or by a combination of the two anywhere in the country are collected at the NCSC for evaluation.
- ✓ There is a team of experts called the Cross Section Working Evaluation Group whose sole and continuous function is to evaluate cross section data for nuclear reactions of neutrons, gammas, and charged particles.
- ✓ Similar teams work in Europe (JEFF) and Japan (JENDL) developing similar sets of data

DATA PROCESSING

- ✓ At BNL, all the information about nuclear cross sections is stored in a huge computer-data library known as the Evaluated Nuclear Data Files (ENDF).
- ✓ There are two types of files, file type A and file type B.
- ✓ The data in file A are, generally, incomplete in terms of their evaluation, and for this reason the information contained there and known as ENDF/A is used only by the specialists who evaluate the cross sections.
- ✓ File B contains the evaluated cross-section data known as ENDF/B, the data used by all persons involved in reactor physics calculations.

DATA PROCESSING

- The evaluated nuclear data files (such as ENDF, JEFF and JENDL) are developed utilizing information from experimental cross-section data; integral data (critical assemblies); and nuclear models and theory.
- Review, compilation, processing, and analysis of uncertainty data for neutron induced reactions available in the most recent different internationally distributed nuclear data libraries have been performed.
- Although the evaluation of nuclear cross sections is a continuous process, for practical reasons, evaluated data are not released to the users on a continuous basis.
- Instead, every few years a new complete version is released for general use.

DATA PROCESSING

The last evaluated nuclear data files available in NEA/OECD and RSICC ORNL are:

- **ENDF/B-VI.8 (2001) and ENDF/B-VII.0 (2007)**
- **JEFF-3.1 (2005)**
- **JENDL-3.3 (2002) – coming soon JENDL-4.0**

AVAILABLE COVARIANCE DATA

Data files	Number of materials	Number of cross-sections
ENDF/B-VI.8	44	400
JEFF-3.1	34	350
JENDL-3.3	20	160

DATA PROCESSING

The official release of ENDF/B-VII.0 has been released at the end of 2006. (National Nuclear Data Center – www.nndc.bnl.gov).

ENDF.B-VII library contains 14 sub-libraries (2-new, 7 – many improvements and updates, 5 – unchanged).

It is the largest library – it contains data for 393 materials (390 isotopes + 3 elements).

For comparison the JEFF-3.1 library contains 381 materials, and the JENDL-3.3 contains 337 materials.

DATA PROCESSING

There are major improvements in the ENDF.B-VII library as compared to the previous versions/releases:

Significant advances in actinide cross-sections

Fission products completely updated.

Includes resonances (resolved and unresolved) in modern representation.

DATA PROCESSING

The following type of information is contained in ENDF/B for more than 200 isotopes, some molecules, and some special mixtures (e.g., some fission products are lumped together as single pseudo-materials) for all known nuclear reactions:

1. **the decay constant;**
2. **type of decay;**
3. **cross-section values, as a function of neutron energy, from very low energies up to 20 Me V, as well as scattering cross section values, as a function of the scattering angle, for the same energy range;**
4. **resonance parameters;**
5. **fission product yields;**
6. **secondary neutron energy and angular distribution (for fission neutrons, this is the value of $\chi(E)$, the fission neutron energy spectrum).**

DATA PROCESSING

- ✓ In the ENDF/B, the cross sections are represented as a combination of tabulated cross sections and resonance parameters.
- ✓ To solve the transport equation in any approximation, cross sections must be defined at all energies.
- ✓ In energy regions where the cross sections are not tabulated, the required cross-section values are obtained with the help of interpolation schemes.
- ✓ The ENDF/B library provides the five interpolation schemes shown in the Table

Table - ENDF Interpolation Schemes

Option	Function
Constant	$\sigma(E) = A$
Linear-linear	$\sigma(E) = A + BE$
Linear-log	$\sigma(E) = A + B\ln(E)$
Log-linear	$\sigma(E) = A\exp(BE)$
Log-log	$\sigma(E) = A \cdot E^{B}$

DATA PROCESSING

- ✓ Experience has shown that the choice of the interpolation law is important because the use of the wrong scheme may produce cross sections that lead to erroneous results when they are subsequently utilized for neutronic calculations.

- ✓ The errors are reduced if linearization schemes are used to represent the cross sections within a range where a particular interpolation law has been used.

- ✓ The resonance parameters are used to reconstruct the cross sections in the energy range where the resonance occurs.

DATA PROCESSING

- This reconstruction is not a trivial matter.
- It may lead to significant errors if performed incorrectly.
- The person who performs this task should take into account if at any particular energy region,
  - there is only one isolated resonance;
  - there are many, but resolved, resonances;
  - there are many, but unresolved, resonances.
- In each of the cases mentioned, the treatment of the resonances is different and, therefore, the resulting cross-section values are also different.

DATA PROCESSING

- ✓ Another problem associated with resonances is the so-called "self-shielding."
- ✓ The term self-shielding is used to describe the following phenomenon: at the resonance energy, where the value of the cross section is extremely high, the neutron flux is depressed.
- ✓ Since the flux is depressed, the number of reactions at that energy also decreases, thus "shielding" the resonance from the neutron flux.
- ✓ The treatment of self-shielding is complicated by the fact that the phenomenon is spatially dependent (it depends on geometry and even on direction).

DATA PROCESSING

- ✓ The user of ENDF/B should remember that the values of cross sections are given under the assumption that neutrons collide with stationary nuclei.
- ✓ In reality, the nuclei have a thermal motion that is important, particularly in the case of resonances.
- ✓ Then, the Doppler effect comes into play and the absorption rate depends on temperature.
- ✓ Since the transport equation describes the neutron population in the laboratory frame of reference and for elevated temperatures, care should be exercised to use the proper cross sections for its solution.

DATA PROCESSING

- ✓ **The ENDF/B library constitutes a tremendous volume of data.**
- ✓ **For the average user utilizing the nuclear cross section data for a reactor physics calculation, starting with ENDF/B represents a monumental task that is not always necessary.**
- ✓ **The overwhelming majority of calculations is performed by applying the multi-group formalism, which does not require all the detail contained in ENDF/B.**

DATA PROCESSING

- For this reason, the common approach taken is to develop sets of group constants for a certain number of groups (~ 40 – 400) that apply to a whole class of problems (e.g., for LWRs, for fast reactors, for AGCRs, etc.).

- To perform a specific calculation, one would choose the cross section set that applies best to the problem and either uses the group constants directly, in a multi-group calculation or, most frequently, produces constants for a smaller number of groups using a process called "cross-section collapsing."

DATA PROCESSING

The development of group constants from the ENDF/B follows these steps:

1. **The transport equation is solved for the neutron energy spectrum $\phi(E)$**
2. **Using the spectrum $\phi(E)$, a set of group constants is computed over a superfine- or fine-group structure. *At this step, the number of groups is more than a thousand. The latest Westinghouse fine-group library contains 6000 groups***
3. **The group constants obtained in step 2 are used for the generation of new constants over a broad-group structure (~40 - 400 groups).**

DATA PROCESSING

The transport equation, in terms of the energy variable alone, takes the form (for a homogeneous medium):

$$\Sigma_t(E)\phi(E) = \sum_{j=1}^{M} \int_{E}^{E/\alpha_j} \frac{\Sigma_s^j(E' \rightarrow E)}{(1-\alpha_j)E'} \phi(E')dE' + S(E)$$

The summation $j = 1, M$ is over all the isotopes present in the medium. The source $S(E)$ is, for a reactor without external sources:

$$S(E) = (1/k)\chi(E) \int_{E'=0}^{E_{\max}} \nu(E')\Sigma_f E')\phi(E')dE'$$

DATA PROCESSING

- ✓ **The solution of this equation is the neutron flux as a function of energy in an infinite homogeneous medium at steady state.**
- ✓ **The properties of the medium enter through the cross sections, the atom concentrations, and the constants**

$$\alpha_j = [(A_j - 1)/(A_j + 1)]^2$$

where A_j is the atomic weight of isotope .

- ✓ **In reality, the codes that solve this equation keep a "mild" space dependence through a buckling B^2, but that detail is not important for our discussion here.**

DATA PROCESSING

- For a heterogeneous medium, the equation for takes a different form because the flux $\phi(E)$ is different in the separate media involved and neutrons may travel from one medium to another.
- As a result, the transport equation is transformed into coupled equations.
- Consider, for example, the usual case of two separate media - fuel and moderator.
- The two equations for the fuel and moderator are:

DATA PROCESSING

$$V_F \Sigma_{tF}(E)\phi_F(E) = V_F[1 - P^0_{F\to M}(E)] \int_E^{E/\alpha_F} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$
$$+ V_M P^0_{M\to F}(E) \int_E^{E/\alpha_M} \phi_M(E')\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE'$$

$$V_M \Sigma_{tM}(E)\phi_M(E) = V_F P^0_{F\to M}(E) \int_E^{E/\alpha_F} \phi_F(E')\Sigma_{sF}(E')\left(\frac{1}{1-\alpha_F}\right)\left(\frac{1}{E'}\right)dE'$$
$$+ V_M[1 - P^0_{M\to F}(E)] \int_E^{E/\alpha_M} \phi_M(E')\Sigma_{sM}(E')\left(\frac{1}{1-\alpha_M}\right)\left(\frac{1}{E'}\right)dE'$$

DATA PROCESSING

where

V_F = volume of fuel;

V_M = volume of moderator;

$P^0_{F\to M}(E)$ = probability that a neutron of energy E escapes from the fuel without a collision in the fuel;

and the rest of the symbols have their usual meaning.

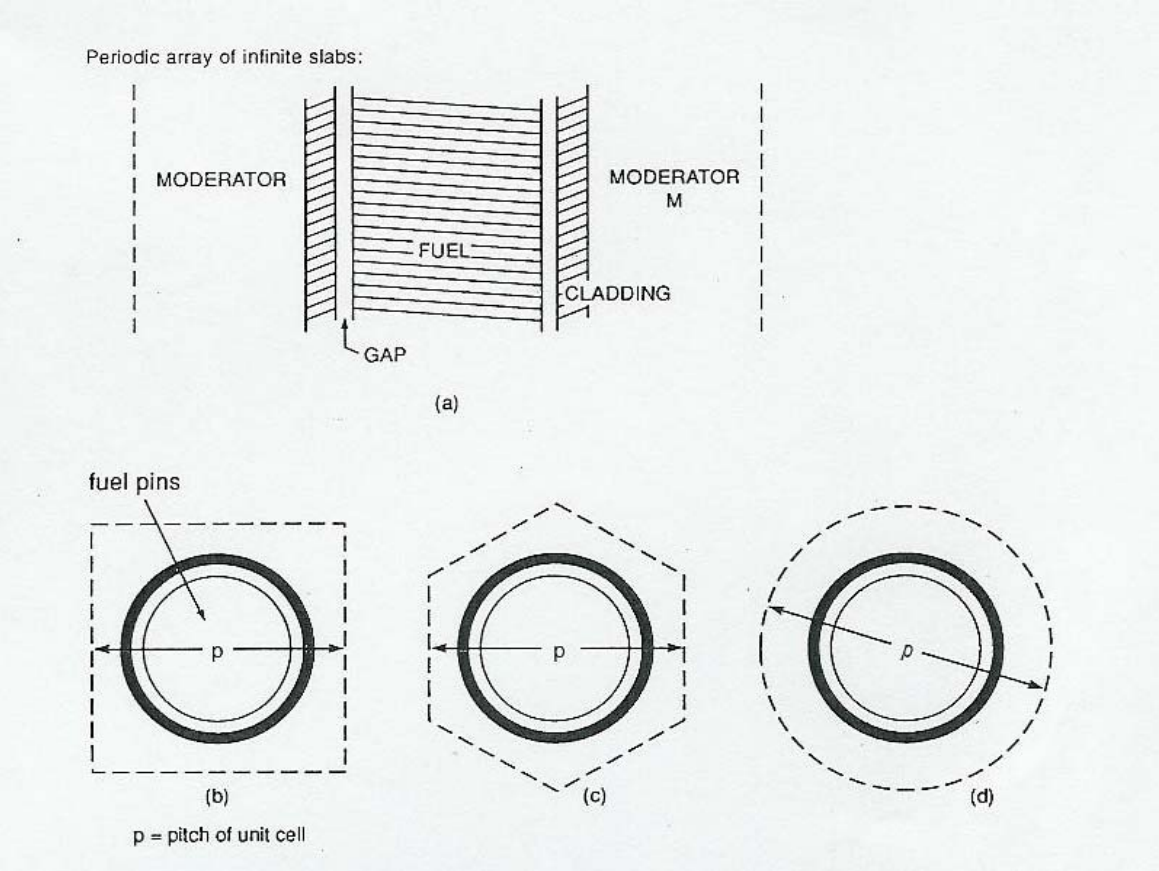
DATA PROCESSING

- ✓ All the cross sections necessary for the solution of these equation are taken directly from ENDF/B.
- ✓ The solution is achieved by numerical techniques.
- ✓ It is not a very difficult problem, but it is not a trivial one either.
- ✓ Since the energy spans seven decades, one has to consider the variation of the cross sections over that same range, which means that the resonances have to be treated properly.

DATA PROCESSING

- ✓ In modeling a reactor for these equations, it is not necessary to consider the whole core.
- ✓ Normally, one chooses a unit cell, which may be regarded as the smallest repeating unit of a reactor core that has the properties of a critical assembly.
- ✓ The use of the unit cell simplifies the calculation considerably, since the alternative would be to model each fuel rod separately.

DATA PROCESSING



Configurations of typical unit cells: (a) plane, (b) square, (c) hexagonal, and (d) cylindrical

DATA PROCESSING

After the neutron energy spectrum $\phi(E)$ is obtained, multi-group constants are computed based on the equation

$$\sigma_h = \frac{\int_{E_h}^{E_{h-1}} \sigma(E)\phi(E)dE}{\int_{E_h}^{E_{h-1}} \phi(E)dE} \quad \Big| h = 1, H$$

for all isotopes and cross-section types.

A set of multi-group constants is known as an input "cross section library" to be used in lattice physics calculations.

DATA PROCESSING

- The group structure at this stage is a "fine" one. It is not unusual for *H* to be equal to a thousand or more groups.

- As mentioned earlier, most reactor calculations are performed with a smaller number of groups, in which case there is a need for new group constants corresponding to the new group structure.

- This task, called cross section collapsing, is accomplished in the following manner.

DATA PROCESSING

- Consider *H* fine groups with energy group boundaries $E_h \big| h = 1, H$ and a new "broad"-group structure consisting of *G* groups with energy group boundaries

$$E_g \big| g = 1, G$$

- A basic requirement in going from *H* to *G* group constants is that the energy boundaries of the *G* groups must coincide with boundaries of the *H* groups
- The system under study is modeled in one dimension and the transport equation is solved in *H* groups, thus providing the fluxes

$$\phi_h(r) \big| h = 1, H$$

DATA PROCESSING

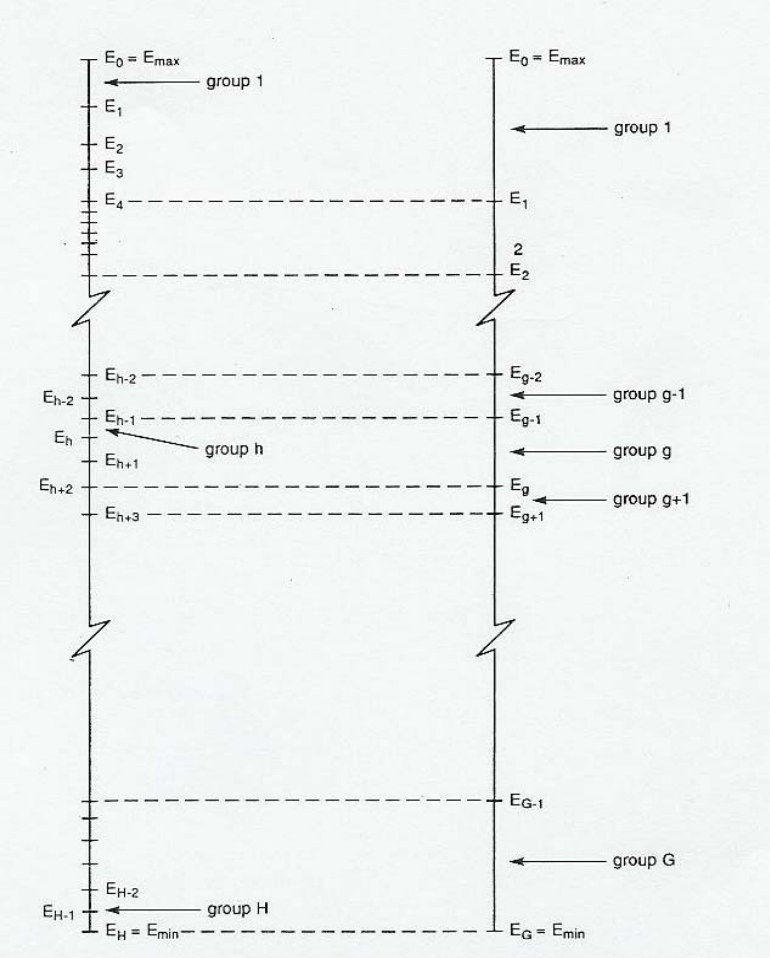
- Any cross section in the broad-group structure is then obtained by

$$\sigma_g(r) = \frac{\sum_h \sigma_h(r)\phi_h(r)(\Delta E)_h}{\sum_h \phi_h(r)(\Delta E)_h} \Big| g = 1, G$$

and $(\Delta E)_h = E_{h-1} - E_h$

- The summation over h covers all the ***h*** groups whose energy boundaries lie within those of that group – $g'th$
- The group constants obtained by the above equation constitute the collapsed set.

DATA PROCESSING



The fine (H-group) and broad (G-group) structure. Boundaries of the G-group structure should coincide with boundaries of the H-group structure.

DATA PROCESSING

- ✓ The *G*-group set is used for lattice physics calculations.
- ✓ Frequently, this broad-group set consists of ~ 40 to 400 groups.
- ✓ If it was derived based on a model of an reactor type of average composition, it may subsequently be used with a more detailed lattice physics model of the particular reactor under study to produce yet another set of group constants for a much smaller number of few groups (anywhere from 2 to ~30).

DATA PROCESSING

- ✓ What is the optimum number of groups one should use?
- ✓ There is no unique answer to that question.
- ✓ The number of groups depends on the objective of the calculation, the reactor type (thermal or fast), the accuracy desired, and the amount of computer time for which one is willing to pay.
- ✓ Later we will discuss a methodology for selection optimal group structures for given type of reactor and particularly for AGCRs

DATA PROCESSING

As mentioned before there exist in the world several sets of evaluated nuclear data which have been both checked for consistency and benchmarked extensively in the calculation of experiments designed for data testing.

Representation of the cross section data in such data files is generally as follows:

1. $\sigma(E_i)$ **are tabulated point-wise in energy at low energies below the resonance region.**
2. **Resolved resonance parameters and background cross sections in the resolved resonance region.**
3. **Unresolved resonance statistical parameters and background cross section in the unresolved resonance region.**
4. $\sigma(E_i)$ **are tabulated point-wise in energy at energies above the resonance region.**
5. **Scattering transfer functions** $p(E_i, \mu_s)$ **are tabulated point-wise in energy and either point-wise in angle** (μ_{sj}) **or as Legendre coefficients.**

DATA PROCESSING

The scattering transfer function - the probability that a neutron will undergo a scattering event which changes its direction from direction Ω to direction Ω'

($\mu_s = \Omega \cdot \Omega'$) and its energy from E to E'- is represented as

$$\sigma_s(\mu_s, E \to E') = m(E)\sigma_s(E)p(E, \mu_s)g(\mu_s, E \to E')$$

DATA PROCESSING

where $m(E) = 1$ for elastic and inelastic scattering, 2 for $(n, 2n)$, ν for fission; $\mathrm{p}(\mathrm{E}, \mu_s)$ is the angular distribution for scattering of a neutron of energy E; and $g(\mu_s, E \rightarrow E')$ is the final energy distribution of a neutron at energy E which has scattered through μ_s

When the scattering angle and energy loss are correlated, as they are for elastic scattering, $g(\mu_s, E \rightarrow E') = \delta(\mu_s - \mu(E, E'))$

DATA PROCESSING

Otherwise, $g(\mu_{si}, E_j \rightarrow E_k^{'})$ is tabulated. The angular distribution may be tabulated as $p(E_i, \mu_{sj})$,or the Legendre components may be tabulated point-wise in energy

$$p_n(E_i) = \int_{-1}^{1} d\mu_s P_n(\mu_s) p(E_i, \mu_s)$$

Where P_n is the Legendre polynomial.

DATA PROCESSING

- ✓ **There are a number of codes, which directly process the evaluated nuclear data files to prepare multi-group cross sections such as NJOY (called as processing codes)**
- ✓ **For example the SCALE package from ORNL has its own processing capability**
- ✓ **These codes numerically calculate integrals of the type**

$$\sigma^{g} = \frac{\int_{E_g}^{E_{g-1}} dE\,\sigma(E)W(E)}{\int_{E_g}^{E_{g-1}} dE\,W(E)}$$

$$\sigma_n^{g\to g'} = \frac{\int_{E_g}^{E_{g-1}} dE\,\sigma(E)W(E) \int_{E_{g'}}^{E_{g'-1}} dE'\,p(E')}{\int_{E_g}^{E_{g-1}} dE\,W(E)}$$

Ultra-fine group structures – thousands of groups
Fine-group structures – hundreds of groups – cell physics
Multi-group structures – (40 – 400) – lattice physics
Few-group structures – (2-30) – core physics

DATA PROCESSING

for a specified weighting function, $W(E)$, which may be a constant: $1/E$, $\chi(E)$, and so on.

- ✓ These codes are used to calculate *fine-group* cross sections in a few hundred groups for thermal reactors or *ultra-fine-group* cross sections in a few thousand groups for fast reactors.
- ✓ These fine- or ultra-fine-group structures are chosen such that the results of calculations using the fine- or ultra-fine-group cross sections are essentially independent of the choice of weighting function, $W(E)$, used in the cross-section preparation.

DATA PROCESSING

- ✓ **Once the fine- or ultra-fine group cross sections are prepared, a fine- or ultra-fine group spectrum (ϕ_g) is calculated for a representative medium.**
- ✓ **The unit cell heterogeneous structure of the region must be taken into account in collapsing the cross-sections**
- ✓ **Resonances must be treated specially.**
- ✓ **This fine- or ultra-fine group spectrum can then be used to weight the fine- or ultra-fine group cross sections to obtain *multi-group group* cross sections for lattice physics analysis**

DATA PROCESSING

$$\sigma^{k} = \frac{\sum_{g \in k} \sigma^{g} \phi_{g}}{\sum_{g \in k} \phi_{g}}$$

$$\sigma_{n}^{k \to k'} = \frac{\sum_{g \in k} \sum_{g' \in k'} \sigma_{n}^{g \to g'} \phi_{g}}{\sum_{g \in k} \phi_{g}}$$

The notation $g \in k$ indicates that the sum is over all fine or ultra-fine groups g within few or many group k.

DATA PROCESSING

- ✓ The few-group cross sections may be calculated for several different large regions in a reactor.
- ✓ They are then used in a few- group diffusion or transport theory calculation of the entire reactor to determine the effective multiplication constant, power distribution, and so on.
- ✓ Because many such calculations must be made, a number of parameterizations of few- and many-group cross sections have been developed to avoid the necessity of making the fine- or ultra fine-group spectrum calculation numerous times.

The Multi-group Equations

- The discretization of the energy variable with the multi-group approximation may proceed from one of several starting points
- The time-dependent fixed source problem, the k eigenvalue equations, or the kinetics equations are all suitable points of departure depending on the application under consideration
- We choose, for our examples, the time-dependent fixed source equation, since it is applicable to both non-multiplying and subcritical systems, while at the same time it can be simply modified by setting $q_{ex} = 0$ and replacing ν by ν/k to obtain the multiplication eigenvalue form
- These two forms of the equations account for the vast majority of transport calculations

The Multi-group Equations

For our starting point, then we choose the following equation:

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)\right]\psi(\vec{r},\hat{\Omega},E)=$$

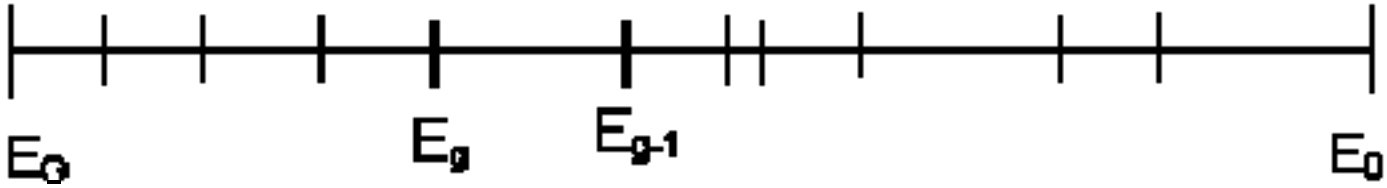
$$q_{ex}(\vec{r},\hat{\Omega},E)+\int_0^\infty d\Omega'\,\sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}\cdot\hat{\Omega}')\psi(\vec{r},\hat{\Omega}',E')$$

$$+\chi(E)\int_0^\infty dE'\,\nu\,\sigma_f(\vec{r},E')\phi(\vec{r},E')$$

where $\phi(\vec{r},E')$ **is the scalar flux**

The Multi-group Equations

- To derive multigroup equations we first divide the energy range into *G* intervals as shown in the Figure, where $E_G = 0$ and E_0 is sufficiently large that the number of particles at higher energies is negligible:



- The particles in group *g* are taken to be just those with energies between E_g and E_{g-1}; hence the group number increases as the energy decreases

The Multi-group Equations

- **Our objective now is to obtain an approximation to the transport equation in terms of the group angular flux**

$$\psi_g(\vec{r},\hat{\Omega}) = \int_g dE\,\psi(\vec{r},\hat{\Omega},E)$$

where for brevity we employ the shorthand notation $\int_g dE = \int_{Eg}^{E_{g-1}} dE$

- **We proceed by dividing the energy integrals into the contributions for each energy group**

$$\int_0^\infty dE' = \sum_{g'=1}^{G} \int_{g'} dE'$$

and integrating between E_g and E_{g-1} to obtain *(next slide)*

The Multi-group Equations

$$\hat{\Omega}\cdot\vec{\nabla}\int_g dE\,\psi(\vec{r},\hat{\Omega},E)+\int_g dE\,\sigma(\vec{r},E)\psi(\vec{r},\hat{\Omega},E)$$

$$=\int_g dE q_{ex}(\vec{r},\hat{\Omega},E)+\sum_{g'=1}^{G} dE\int_{g'} dE'\int d\Omega'\,\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}',E')$$

$$+\int_{g'} dE\chi(E)\sum_{g'=1}^{G}\int_{g'} dE'\nu\sigma_f(\vec{r},E')\phi(\vec{r},E')$$

- To express this equation in terms of the group fluxes we may proceed in one of two ways
- We may either assume that the angular flux is separable in energy, or we may use the more elegant treatment of Bell, Hansen, and Sandmeir
- We discuss the flux separability approximation first

The Multi-group Equations - Energy Separability

- **Suppose that within each energy group the angular flux can be approximated as the product of a known function of energy *f(E)* and the group $\psi_g(\vec{r},\hat{\Omega})$:**

$$\psi(\vec{r},\hat{\Omega},E) \approx f(E)\psi_g(\vec{r},\hat{\Omega}), \qquad E_g < E \le E_{g-1}$$

where the energy-dependent spectral weighting function *f(E)* is normalized by the definition of the group flux to

$$\int_g dE\, f(E) = 1$$

- **To proceed, we substitute and obtain:**

$$\hat{\Omega}\cdot\vec{\nabla}\psi_g(\vec{r},\hat{\Omega}) + \int_g dE\, f(E)\sigma(\vec{r},E)\psi_g(\vec{r},\hat{\Omega})$$

$$= \int_g dE q_{ex}(\vec{r},\hat{\Omega},E) + \sum_{g'=1}^{G} dE \int_{g'} dE' \int d\Omega' \sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega}) f(E')\psi_{g'}(\vec{r},\hat{\Omega}')$$

$$+ \int_{g'} dE \chi(E) \sum_{g'=1}^{G} \int_{g'} dE' \nu\sigma_f(\vec{r},E') f(E')\phi_{g'}(\vec{r})$$

The Multi-group Equations - Energy Separability

- **If we define the multigroup cross-sections as:**

$$\sigma_g(\vec{r}) = \int_g dE\, \sigma(\vec{r}, E) f(E)$$

$$\nu\sigma_{fg}(\vec{r}) = \int_g dE\, \nu\sigma_f(\vec{r}, E) f(E)$$

$$\sigma_{gg'}(\vec{r}, \hat{\Omega}'\cdot\hat{\Omega}) = \int_g dE \int_{g'} dE'' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}'\cdot\hat{\Omega}) f(E')$$

and let

$$\chi_g = \int_g dE\, \chi(E)$$

$$q_g^e(\vec{r}, \hat{\Omega}) = \int_g dE\, q_{ex}(\vec{r}, \hat{\Omega}, E)$$

(next slide)

The Multi-group Equations - Energy Separability

- **We arrive to the conventional multigroup form:**

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g(\vec{r})\right]\psi_g(\vec{r},\hat{\Omega})=\sum_{g'=1}^{G}\int d\Omega'\,\sigma_{gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}')$$

$$+\chi_g\sum_{g'=1}^{G}\nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})+q_g^e(\vec{r},\hat{\Omega})$$

- **The boundary conditions to be used in conjunction with the foregoing multigroup equations are the same as those described for continuous energy, with exception that** $\psi(\vec{r},\hat{\Omega},E)$ **is replaced by** $\psi_g(\vec{r},\hat{\Omega})$

- **Before proceeding to other forms of the transport equations we note that we may obtain a multigroup balance equation, analogous to the continuous energy form**

The Multi-group Equations - Energy Separability

- To obtain this balance condition we integrate the last equation over angle to yield

$$\vec{\nabla}\cdot\int d\Omega\,\hat{\Omega}\psi_g(\vec{r},\hat{\Omega})+\sigma_g(\vec{r})\int d\Omega\,\psi_g(\vec{r},\hat{\Omega})$$

$$=\sum_{g'}\int d\Omega'\left[\int d\Omega\,\sigma_{gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\right]\psi_{g'}(\vec{r},\hat{\Omega}')$$

$$+\chi_g\sum_{g'=1}^{G}\nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})+\int d\Omega\,q_g^e(\vec{r},\hat{\Omega})$$

- We define the group current as $\vec{J}_g(\vec{r})=\int d\Omega\,\hat{\Omega}\psi_g(\vec{r},\hat{\Omega})$

  and the group external source as $q_g^e=\int d\Omega\,q_g^e(\vec{r},\hat{\Omega})$

The Multi-group Equations - Energy Separability

- **The bracketed integral on the right of the equation is just equal to the group-to-group scattering cross-sections:**

$$\sigma_{gg'}(\vec{r}) = \int d\Omega \sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega})$$

- **Hence we may express the balance equation as**

$$\vec{\nabla} \cdot \vec{J}_g(\vec{r}) + \sigma_g(\vec{r})\phi_g(\vec{r}) = \sum_{g'} \sigma_{gg'}(\vec{r})\phi_{g'}(\vec{r}) + \chi_g \sum_{g'} \nu \sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) + q_g^e(\vec{r})$$

- **If we assume that Fick's law is a reasonable approximation,**

$$\vec{J}_g(\vec{r}) = -D_g(\vec{r})\vec{\nabla}\phi_g(\vec{r})$$

where $D_g(\vec{r})$ are group diffusion coefficients, then the balance condition leads to the multigroup diffusion equations *(next slide)*

The Multigroup Equations - Energy Separability

$$\left[-\vec{\nabla}D_g(\vec{r})\cdot\vec{\nabla}+\sigma_g(\vec{r})\right]\phi_g(\vec{r})=\sum_{g'}\sigma_{gg'}(\vec{r})\phi_{g'}(\vec{r})+\chi_g\sum_{g'}\nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})+q_g^e(\vec{r})$$

- Just as this an approximation to the multigroup transport equations we must derive approximations to the boundary conditions on $\psi_g(\vec{r},\hat{\Omega})$

- It is left as an exercise to show that Fick's law implies that on a reflective boundary $\hat{n}\cdot\vec{\nabla}\phi=0$, where $\hat{n}$ is normal to the boundary, and on a vacuum boundary $\hat{n}\cdot\vec{\nabla}\phi+2D_g(\vec{r})\phi(\vec{r})=0$

- Analogous to the continuous energy forms of the transport equation, the differential scattering cross-section appearing in the scattering term of the multigroup equation is frequently expressed as a Legendre expansion

The Multi-group Equations - Energy Separability

- **Thus inserting the equation**

$$\sigma_s(\vec{r}, E' \to E, \mu_0) = \sum_{l=0}^{\infty} (2l+1)\sigma_{sl}(\vec{r}, E' \to E) P_l(\mu_0)$$

into

$$\sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \int_g dE \int_{g'} dE'' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) f(E')$$

we obtain

$$\sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \sum_{l=0}^{\infty} (2l+1)\sigma_{\mathrm{lg}g'}(\vec{r}) P_l(\hat{\Omega}' \cdot \hat{\Omega})$$

where the orthogonality properties of the Legendre polynomials allow us to write

$$\sigma_{gg'}(\vec{r}) = \int_g dE \int_{g'} dE' \sigma_{sl}(\vec{r}, E' \to E) f(E')$$

The Multi-group Equations - Energy Separability

- **The Equation**

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g(\vec{r})\right]\psi_g(\vec{r},\hat{\Omega})=\sum_{g'=1}^{G}\int d\Omega'\,\sigma_{gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}')$$

$$+\chi_g\sum_{g'=1}^{G}\nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})+q_g^e(\vec{r},\hat{\Omega})$$

is the multigroup analog to the continuous energy form

$$[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E)$$

$$=q_{ext}(\vec{r},\hat{\Omega},E)+\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E')$$

$$+\chi(E)\int dE'\,\nu\sigma_f(\vec{r},E')\int d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',E'),\qquad \vec{r}\in V$$

The Multi-group Equations - Energy Separability

- **The multiplication eigenvalue form of the multigroup equation, obtained by setting the external source to zero and replacing *v* by *v/k*, for example, becomes**

$$[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g(\vec{r})]\psi_g(\vec{r},\hat{\Omega})$$

$$=\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}')+\frac{1}{k}\chi_g\sum_{g'=1}^{G}\nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})$$

- **Similarly, the multigroup neutron kinetics equation may be shown to be**

$$\left[\frac{1}{v_g}\frac{\partial}{\partial t}+\hat{\Omega}\cdot\vec{\nabla}+\sigma_g(\vec{r})\right]\psi_g(\vec{r},\hat{\Omega},t)$$

$$=\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}'t)+\chi_{pg}\sum_i(1-\beta^i)\sum_{g'=1}^{G}\nu\sigma^i_{fg'}(\vec{r})\phi_{g'}(\vec{r},t)$$

$$+\sum_l\chi_{1g}\lambda_l C_l(\vec{r},t)+q^e_g(\vec{r},\hat{\Omega})$$

The Multi-group Equations - Energy Separability

and for six groups of delayed neutrons

$$\frac{\partial}{\partial t}C_l(\vec{r},t)=\sum_i \beta_l^i \sum_{g'=1}^{G} \nu\sigma_{fg'}^{i}(\vec{r})\phi_{g'}(\vec{r},t)-\lambda_l C_l(\vec{r},t), \qquad i=1,\ldots 6$$

- **In the former equation, it is assumed that**

$$\int_g dE \frac{1}{\upsilon}\frac{\partial \psi}{\partial t}=\frac{1}{\upsilon_g}\frac{\partial \psi_g}{\partial t}$$

and thus

$$\frac{1}{\upsilon_g}=\int_g dE \frac{1}{\upsilon} f(E)$$

Multi-group cross-section evaluation

- Before multigroup transport calculations can be carried out, values of the multigroup cross-sections must be available
- However, the evaluation of group cross-sections require that both the detailed energy dependence of the cross-sections and the spectra; weighting function $f(E)$ be known
- The energy dependence of the microscopic cross-sections is becoming available with ever increasing accuracy through evaluated data files, such as ENDF for neutrons.
- The evaluation of $f(E)$ is a more subtle matter, for it depends a great deal on characteristics of the system under analysis, and in particular on the analytical and/or computational models that are available for description of that system

Multi-group cross-section evaluation

- The details of cross-section evaluations are treated extensively in texts on shielding and reactor physics
- In many cases the techniques are similar whether the multigroup equations are employed in the transport equation or its diffusion approximation
- While the evaluation of cross-sections was discussed in previous slides, the general remarks that follow may be instructive in summarizing some of the considerations that typically arise in generating multi-group cross-sections for transport calculations

Multi-group cross-section evaluation

- If an exceedingly fine-energy-group structure can be used, analytic or semi-analytic approximations for $f(E)$ may be adequate

- The simplest of these is to take $f(E)$ to be constant,

$$f(E) = \frac{1}{\Delta E_g}, \qquad E_g \le E \le E_{g-1}$$

  where $\Delta E_g \equiv E_{g-1} - E_g$ assures that the normalization condition is met

- Then $\sigma_g(\vec{r}) = \frac{1}{\Delta E_g} \int_g dE \sigma(\vec{r}, E)$ and the group cross-sections depend only on the energy-dependent cross-sections

Multi-group cross-section evaluation

- **For cross-sections with smooth energy dependence, weighing factors in which $f(E) \propto 1/E$ or $1/[E\sigma(E)]$ can be more easily justified on analytical ground**
- **Where the cross-section has the resonance structure of the neutron cross-section, the foregoing recipes are most often inadequate even for very fine energy group discretization**
- **In these cases the flux depression called energy self-shielding through the resonance energy must be taken into account trough more sophisticated methods, such as the narrow and wide resonance methods**
- **More sophisticated methods are also necessary to take into account the effects of thermalization in neutron transport, of Compton edges in gamma ray calculations, and of other phenomena**

Multi-group cross-section evaluation - Infinite medium

- The expense of solving multigroup transport problems often precludes the use of a number of energy groups that is large enough for the semi-analytic modeling of $f(E)$ to be adequate
- As a result it is common to first perform an infinite medium fine-energy-group calculation in which the spatial dependence is eliminated
- From the result of such a calculation, an approximation for $f(E)$ within each of the coarser energy groups can be obtained
- The coarser energy group cross-sections are then obtained by appropriately collapsing the fine-group results

Multi-group cross-section evaluation - Infinite medium

- To illustrate, let us assume that the neutron flux is in an infinite medium and has no spatial or angular dependence

- The scattering term then vanishes, and we can integrate over all angles to obtain infinite medium multigroup equations in terms of the scalar flux:

$$\sigma_j^* \phi_j^* = \sum_{j'} \sigma_{jj'}^* \phi_{j'}^* + \frac{\chi_j^*}{k} F$$

where

$$F \equiv \sum_{j'} \nu\sigma_{jj'}^* \phi_{j'}^*$$

We hereafter use the subscript *jj'* to denote the fine-group indices and the superscript * to denote the fine-group quantities of the problem

Multi-group cross-section evaluation - Infinite medium

- Since we need only the relative magnitudes of the fine-group fluxes, we are not interested in the values of k or F

- Thus we can take $F/k = 1$ creating a fixed source problem, and allowing the previous equation to solve for the ϕ_j^*

- Then within the broader energy group we can define $f(E)$ as the normalized step function

$$f(E) = \frac{\phi_j^*}{\sum_{j' \in g} \phi_{j'}^*}, \qquad E_j < E < E_{j-1}, \quad j \in g$$

where $j \in g$ includes only those fine groups lying within the broad group g; i.e., for which $E_g \le E_j < E_{j-1} \le E_{g-1}$

Multi-group cross-section evaluation - Infinite medium

- With $f(E)$ known, the fine-group cross-sections can be collapsed to broader group cross-sections

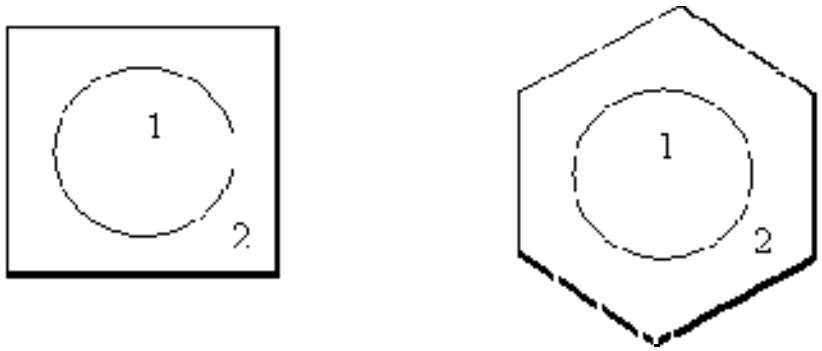
- For example, the equation $\sigma_g(\vec{r}) = \int_g dE\, \sigma(\vec{r}, E) f(E)$

  is approximated by

$$\sigma_g(\vec{r}) = \frac{\sum_{j \in g} \phi_j^* \sigma_j^*(\vec{r})}{\sum_{j \in g} \phi_j^*}$$

Multi-group cross-section evaluation - Lattice Cell

- There are at least two important situations where the use of fine-group infinite medium calculations for the generation of broader group cross-sections is inadequate
- The first of these arise frequently in reactor lattice calculations
- Such a calculation may have as its spatial domain many units cells, each consisting of fuel and coolant in separated regions and arranged in a periodic array
- Two simplified two-region unit cell configurations are depicted below



Multi-group cross-section evaluation - Lattice Cell

- In most cases the computational cost of treating the heterogeneous structure of each cell explicitly within a larger many-cell problem would be prohibitive
- Thus the cell cross sections are homogenized to cell-averaged values
- In case where the cell dimensions are small in mean free paths, simple volume averages may be acceptable
- Often, however, the true flux may exhibit sufficiently large spatial variation between the regions of the cell that it must be accounted for in the homogenization procedures

Multi-group cross-section evaluation - Lattice Cell

- The most common procedure for accounting for cell flux variation in group cross-sections may be illustrated in terms of the simple two-region cells
- Calculations are based on an infinite lattice problem in which reflective conditions are imposed at all of the cell boundaries
- These provide fine energy mesh values of ϕ^*_{j1} and ϕ^*_{j2}, the volume-averaged flux values in each of the cell regions
- A wide variety of methods have been applied for such purposes ranging from semi-analytic approximations for the flux ratios to the use of numerical transport methods

Multi-group cross-section evaluation - Lattice Cell

- **Knowing the flux value and the fine-group region cross-sections, σ^*_{j1} and σ^*_{j2} , homogenized cross-sections, averaged over fine groups, may be obtained**

- **For example, the group total cross-section is**

$$\sigma_g(\vec{r}) = \frac{\sum_{j\in g}\left(V_1\sigma^*_{j1}\phi^*_{j1} + V_2\sigma^*_{j2}\phi^*_{j2}\right)}{\sum_{j\in g}\left(V_1\phi^*_{j1} + V_2\phi^*_{j2}\right)}$$

Multi-group cross-section evaluation - Buckling Corrections

- A second situation where the use of fine-group infinite medium calculations for evaluation of multigroup cross-sections may arise is when the overall dimensions of the system are not large, for large net leakage of neutrons may then cause a significant distortion of the infinite medium fine-group distribution

- For homogeneous media this leakage may ne roughly accounted for by assuming the approximation

$$\psi_j^*(\vec{r},\hat{\Omega}) = \psi_j^*(\hat{\Omega})\exp[i\vec{B}\cdot\vec{r}]$$

where $B = \left|\vec{B}\right|$ is the buckling familiar from elementary reactor theory

Multi-group cross-section evaluation - Buckling Corrections

- **The buckling is chosen to be the lowest eigenvalue of the Helmholtz equation**

$$\nabla^2\phi + B^2 = 0$$

where $\phi = 0$ on the extrapolated boundaries and $\phi > 0$ within the reactor

- **Hence *B* increases and the leakage correction becomes larger as the size of the system decreases**

Multi-group cross-section generation

- The multi-group cross sections are very important data for the nuclear reactor analyses
- Standard cross-section generation techniques involve three major steps
- The first one is to generate a fine-group cross-section library from the ENDF/B data using a piecewise linear energy weighting function generated from theoretical spectrum approximations

Multi-group cross-section generation

- The cross sections are processed with the appropriate resonance treatment method
- Second, infinite array unit cell calculations using the fine-group library are performed to get the spatial flux distribution
- These weighting flux functions are used to collapse the fine-group library to a broad-group library
- The third step involves spatial homogenization of the unit cell in the framework of the broad group structure

Multi-group cross-section generation

- **The NJOY code is used for cross section processing followed with the AMPX module from the SCALE code package for post-processing of cross sections.**

- **The standard cross section generation procedure contains several steps as follows:**

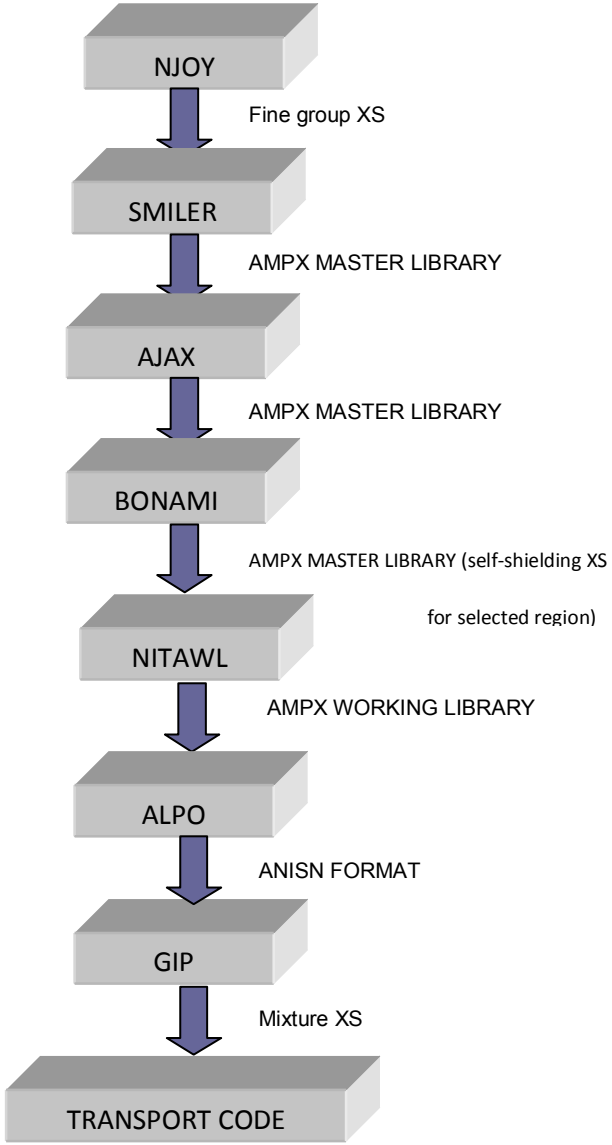
  - **Step 1: NJOY generates multi-group cross section in Group-wise Evaluated Nuclear Data Format (GENDF) format.**

  - **Step 2: SMILER converts the NJOY (GENDF) files to the AMPX master library format**

Multi-group cross-section generation

- **Step 4: BONAMI performs resonance self-shielding effect with Bondarenko factors**
- **Step 5: NITAWL converts AMPX master library to AMPX working library format**
- **Step 6: ALPO converts AMPX working library format to standard ANISN format**
- **Step 7: GIP generates mixture cross-section library.**
- **Step 8: Utilize the multi-group cross section library with a transport code**

Multi-group cross-section generation



Multi-group cross-section generation

- The accuracy of a set of multi-group constants is determined by the selected energy group structure and the utilized weight function.

- It is necessary to have a weight function that represent as accurate as possible the flux distribution as a function of energy in the nuclear reactor core of interest.

- GROUPR in NJOY provides the in-code built weight functions that represent a few typical nuclear systems including the thermal reactor spectrum.

Multi-group cross-section generation

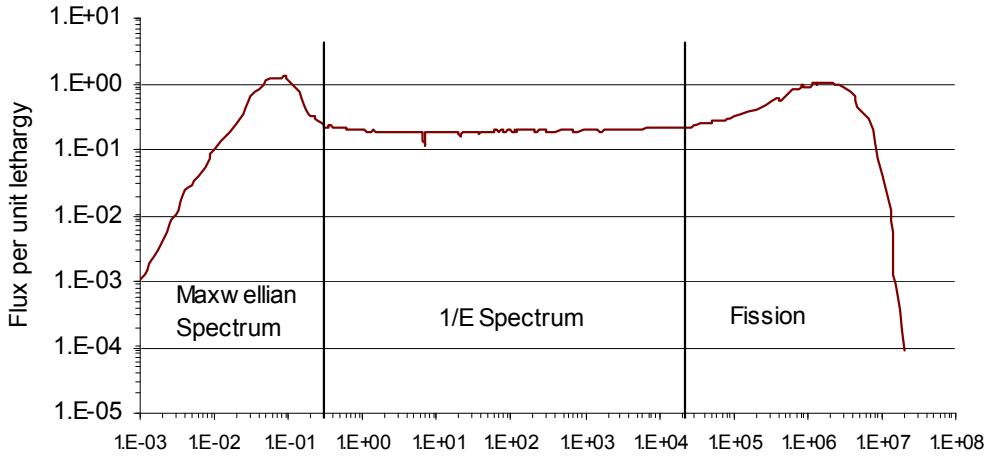
- The later weight function combines a thermal Maxwellian at low energies, a 1/E function at intermediate energies, and a fission spectrum at high energies.

- In GROUPR, user has freedom to choose the temperatures of the Maxwellian and fission parts and the energies where the spectra join.

- For example the cutoff energies between spectra can be determined by using the Maxwell-Boltzmann distribution function for low energies and a 1/E function for intermediate energies

Multi-group cross-section generation

- **As a result, the function consists of:**
  - **A Maxwellian spectrum (peak at 0.07eV) from 10^{-5} to 0.3 eV**
  - **An 1/E spectrum from 0.3 eV to 20.0 keV**
  - **A fission spectrum from 20.0 keV to 20 MeV.**



Multi-group cross-section generation

- One of the most important issues to be considered in criticality calculations is the energy self-shielding in the resonance region for multi-group cross sections

- The method utilized for treatment of energy self-shielding is one of the factors in a multi-group cross-section generation that may have a significant impact on the multiplication factor and also on the absorption reaction rate predictions, mostly in the epithermal region.

- In the “resonance energy” region, from roughly 1 eV to 100 keV, the main absorption of neutrons by heavy nuclei takes place at pronounced peaks or resonances of cross section

Multi-group cross-section generation

- The shielding effects are presented in this region because of the flux dip at resonances
- The resonance structure can be separated into two regions, resolved and unresolved
- In resolved resonance region, the resonances are wide when compared to the scattering ranges for the mixtures in a particular configuration
- It is in the range of eV up to a few keV. This region is significant for thermal reactors.

Multi-group cross-section generation

- In the unresolved resonance region, the resonances are not able to achieve adequate resolution of the individual resonances
- The neutron absorption in this region is important for fast reactors
- An appropriate treatment of the resonance absorption is needed in order to obtain more accurate solutions
- Three methods for resonance shielding treatment are explained

❑ Flux Calculator

- ➢ **The narrow resonance approach is quite useful for practical fast reactor problems.**
- ➢ **However, for nuclear systems sensitive to energies from 1 to 500 eV, there are many broad- and intermediate-width resonances, which cannot be self-shielded with sufficient accuracy using the Bondarenko approach.**
- ➢ **The flux calculator option of GROUPR module in NJOY is designed to solve such problems.**

- **The infinite-medium neutron spectrum equation is expressed as:**

$$\Sigma_t(E)\Phi(E) = \int_0^\infty dE' \Sigma_s(E' \to E)\Phi(E') + S(E)$$

where the term on the left hand side of the Equation represents the collision, the integral on the right hand side is the scattering source, and S(E) the external source.

- **Next, the Equation is written considering a homogeneous medium consisting of two materials: an absorber and a moderator, represented by A and M**

- Elastic scattering cross sections that are isotropic in the center of mass are used

- Neutron slowing down in a single resonance of the absorber material is assumed

$$\Sigma_t(E)\Phi(E) = \int_E^{E/\alpha_M} dE' \frac{\Sigma_s^M(E')}{(1-\alpha_M)E'}\Phi(E') + \int_E^{E/\alpha_A} dE' \frac{\Sigma_s^A(E')}{(1-\alpha_A)E'}\Phi(E')$$

where α_M and α_A are the moderator and absorber collision parameters, respectively, defined as:

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$

Multi-group cross-section generation

- **The following approximations are introduced**

  - **The moderator scattering cross-section is assumed to be constant and equal to the potential scattering cross-section: i.e.** $\Sigma_s^M(E') = \Sigma_p^M$

  - **The moderator absorption cross-section is assumed to be negligible; i.e.**

$$\Sigma_t^M(E') = \Sigma_p^M$$

  - **The narrow resonance approximation is used for the moderator.**

  - **This states that the resonance width is very small compared to the energy loss from scattering with the moderator nucleus. scattering cross sections that are isotropic in the center of mass are used**

  - **Neutron slowing down in a single resonance of the absorber material is assumed**

Multi-group cross-section generation

- **This states that the resonance width is very small compared to the energy loss from scattering with the moderator nucleus.**
- **Therefore, the flux distribution is the moderator integral is assumed to have an asymptotic form. In general, the moderator integral is assumed to be a smooth function of energy represented as C(E).**
- **The moderator is assumed to represent all nuclides other than the absorber.**
- **This enables the inclusion of the dilution microscopic cross-section of the absorber, σ_o**
- **The dilution (or background) cross section of an isotope *i* is defined to be all cross sections representing isotopes other than the isotope *i*.**

Multi-group cross-section generation

- **The dilution cross-section is a measure of energy self-shielding**
- **It determines the significance of a resonance compared to other cross sections. If the dilution cross-section (σ_o) is small, it indicates that the resonance has a significant impact on the flux and a large self-shielding effect exists**
- **If σ_o is very large (infinite dilution), the cross sections of the absorber do not affect the flux spectrum, and the flux may be represented as a smooth function of energy.**

$$\left[\sigma_o + \sigma_t^A(E)\right]\Phi(E) = C(E)\sigma_o + \int_E^{E/\alpha_A} dE' \frac{\sigma_s^A(E')}{(1-\alpha_A)E'}\Phi(E')$$

$$\sigma_o = \frac{1}{\rho_i}\sum_{j\neq i}\rho_j\sigma_t^j$$

Multi-group cross-section generation

- **Where *i* and *j* represent isotope indexes and ρ is atomic density.**
- **The above Equation is the simplest form used in NJOY for computing the flux with the flux calculator option**
- **In NJOY, several dilution cross sections are provided as input.**
- **Depending on a system of interest, the cross sections corresponding to the appropriate dilution cross-section are used.**

The Bondarenko Method

- The Bondarenko method is obtained by using the narrow resonance approximation in the absorber scattering integral , which is derived from neutron slowing down equation

$$\left[\sigma_o + \sigma_t^A(E)\right]\Phi(E) = C(E)\sigma_o + \int_E^{E/\alpha_A} dE' \frac{\sigma_s^A(E')}{(1-\alpha_A)E'}\Phi(E')$$

- The practical width of a resonance of the absorber is considered to be much smaller than the energy loss due to a collision with the absorber

- This enables the absorber integral to be represented as a smooth function of energy. Therefore, the flux is represented by:

$$\Phi(E) = \frac{C(E)}{\left(\sigma_t^A(E) + \sigma_o\right)}$$

The Bondarenko Method

- If is larger than the tallest peaks in , the weighting flux ϕ is approximately proportional to the smooth weighting function C(E)
- This is called infinite dilution; the cross section in the material of interest has little or no effect on the flux.
- On the other hand, if is small with respect to , the weighting flux will have large dips at the locations of the peaks in , and a large self-shielding effect will be expected.
- This treatment is good for the unresolved region (high energy resonances) since resonance width in this region is very small.

❑ CENTRM

- **CENTRM (Continuous Energy Transport Module) is the new method existing in SCALE 5.0/SCALE 6.0**

- **It computes continuous-energy neutron spectra in zero- or one-dimensional systems, by solving the Boltzmann Transport Equation using a combination of point-wise and multi-group nuclear data.**

- **Several calculation options are available, including discrete ordinates in slab, spherical, or cylindrical geometry; collision probabilities in slab or cylindrical coordinates; and zone-wise or homogenized infinite media.**

- **In SCALE, CENTRM is used mainly to calculate problem-specific fluxes on a fine energy mesh (>10000 points), which may be used to generate self-shielded multi-group cross section for subsequent criticality or shielding analysis.**

Multi-group cross-section generation

- **CENTRM avoids many of the inherent assumptions by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment**
- **Effects from overlapping resonances, fissile material in the fuel and surrounding moderator, and inelastic level scattering are explicitly handled in CENTRM**
- **Another advantage of CENTRM is that it can explicitly model rings in a fuel pin to more precise model the spatial effect on the flux and cross sections**
- **CENTRM enables problem-dependent multigroup cross sections to have the flexibility and accuracy of pointwise-continuous-energy cross sections for criticality analyses.**

Resonance Scattering Model

- **In today's formulation of the transport equation the scattering is divided into two parts, thermal range (usually below few electron-volts) and epithermal range**
- **At thermal range the interaction of neutrons with matter is modeled taking into account thermal agitation of the atoms and their chemical binding effects**
- **In thermal range, neutrons will lose or gain energy after collision with atoms: slowing-down and up-scattering effects**
- **For light isotopes such as hydrogen in water, a quantum mechanics model is usually used, that leads to well known transfer kernel scattering matrices $S(\alpha, \beta)$**

Resonance Scattering Model

- **In epithermal range, model used in existing codes simply assumes an elastic scattering with no binding effect derived from the classical mechanics kinematics collision theory**
- **Leads to an asymptotic scattering transfer kernel that is where is the initial energy of the neutron before the collision**
- **Classical model assumes neutron energy is far greater than atom's chemical binding energy that can be neglected – supposes target atoms are at rest**
- **In early 90s, a new physical phenomenon that occurs during the neutron slowing down process was discovered**
  - Revealed possibility of neutrons to gain energy during scattering with heavy resonant isotopes in resonance energy range – in the epithermal range
- **A model, called Resonance Scattering Model (RSM) was proposed – since then, many other researchers have proved its theoretical soundness**

Resonance Scattering Model

RSM Revealed Three Important Facts:

1. Strong dependence of shape of transfer kernel on the resonance scattering cross-sections profile, i.e. shape is far from being asymptotic when the initial neutron energy is in the vicinity of the resonance peak,
2. Possibility of neutron up-scattering even at high energy,
3. Strong dependency on temperature of scatters target, i.e. fuel

- **This model has never been used in deterministic core simulations**
  - Implementation in a Monte Carlo code has been attempted, but application was limited to an isolated one pin cell or using continuous Monte Carlo without full implementation of the model for all isotopes, except ^{238}U
- **In a joint PSU/INL project the focus is on changing the kernel of the neutron transport equation solved to predict neutron flux in the reactor core to account for this phenomenon and evaluate its effect on innovative new AGCRs and Deep Burn HTR designs**
- **Implementation is accomplished using deterministic transport solution and multi-group method**

Resonance Scattering Model

- The nuclides of interest include each of the fissile/fissionable nuclides used as fuel in the AGCRs and HTR Deep Burn concept as well as other heavy nuclides that result from the high burn-up levels achieved in the reactor and in the feed
- Heavy nuclides, such as the U, Pu and minor actinide nuclides, will be present in the AGCRs and Deep Burn type reactor in quantities substantially larger than those expected in light water reactors
- Generated data will allow proper accounting of physical properties of nuclides leading to high-fidelity modeling

Resonance Scattering Model

- For the heavy isotopes such as the actinides, a free gas model is used in conjunction with a corrected temperature that takes into account the crystal solid structure of the fuel
- Model changes the way neutrons are interacting with fuel isotopic composition – as a result changes flux spectrum in core that in turn affects absorption and production of neutrons in fuel assemblies
- New differential scattering cross-section kernel was derived using free-gas model with Maxwellian velocity distribution taking into effect dependency on energy of scattering cross-section for heavy isotopes
- Formulation of scattering kernel becomes a convolution (in mathematical sense) of two distributions: the Maxwellian distribution and the scattering cross-section

Resonance Scattering Model

- Recently published experimental results demonstrate that the Free Gas model is experimentally proven to be sufficiently accurate and captures major effects
- Experiment proved that free gas model is good at low temperatures
- At high temperatures (reactor conditions) the model is expected to be even more accurate because at such conditions the neutrons behave more like a free gas
- These facts are very important and show that this model can be used for production calculations, i.e. it is ready to be implemented in design codes – no need for complex solid state models
- After implementation of Free Gas model different approximations to treat solid state effects in neutron-crystal interactions will be studied for further improvement of the RSM
- The will be used to generate scattering matrices for different anisotropic scattering degrees for multi-group transport calculation

Resonance Scattering Model

- **New Resonance Scattering Model (RSM) model is developed:**
  - Equations of new differential scattering cross-section transfer kernel for multi-group applications are derived
  - Challenge is treatment of angular variable (anisotropic scattering) to generate anisotropic scattering kernel
  - Numerical aspect to compute and store matrices is addressed
  - Program code is designed to implement the Resonance Scattering Model (RSM) model
  - New module will be implemented in the NJOY code
- **Modeling tools:**
  - ENDF-B/VI-8 and ENDF-B/VII-0, and NJOY99 nuclear data processing system
  - Cross-section generation codes COMBINE-7 and DRAGON-4
  - PSU core simulator NEM (has three core modeling options in 3-D geometry – Cartesian, Hexagonal-Z – for HTR prismatic design, and Cylindrical – for HTR pebble bed design)
  - MCNP5 and the PSU coupled Monte Carlo based depletion code system PSU-MCOR

Resonance Scattering Model

The first step was to develop the equations in details of the new differential scattering cross-section transfer kernel (as shown below for anisotropic scattering):

$$\sigma_{sn}^{T}(E \to E') = \frac{\beta^{5/2}}{4E}\exp(E/kT)\int_0^{\infty} t\,\sigma_s^{tab}\left(\frac{kT}{A}t^2\right)\times\exp\left(-t^2/A\right)\psi_n(t)dt$$

Where β = (A + 1)/A, A – nucleus mass/neutron mass

$$t = \left[m(A+1)/(2kT)\right]^{1/2}u$$

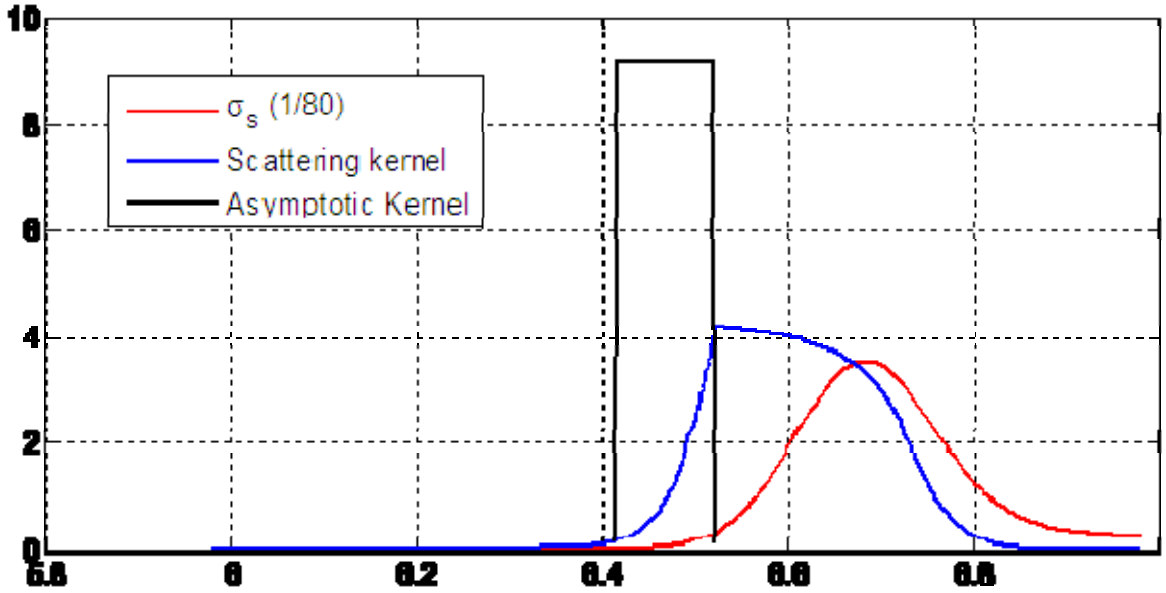
$$x = \left[m(A+1)/(2kT)\right]^{1/2}c$$

Resonance Scattering Model

- In order to verify the scattering kernel formulations derived in the previous slide, neutrons were started at various energies and temperatures and the corresponding scattering kernels were plotted.
- A program has been written to test the formulations derived in the previous section.
- Cross-section values for σ_s^{stab} were generated by NJOY99.161 and interpolated from a linear piecewise continuous tabulation.
- The following Figures illustrate the result of the transfer kernel for ^{238}U (A=238.050785) at 1000 K near the scattering resonances at 6.67 and 36.67eV.
- In each figure the scattering transfer kernels before and after the resonance was calculated.
- In all of the figures it can be seen that the resonance modifies the shape of the transfer kernel with an increase in probability for upscattering for energies at higher temperature.
- This means an increase in absorption which has a direct effect on the reactivity of a reactor.

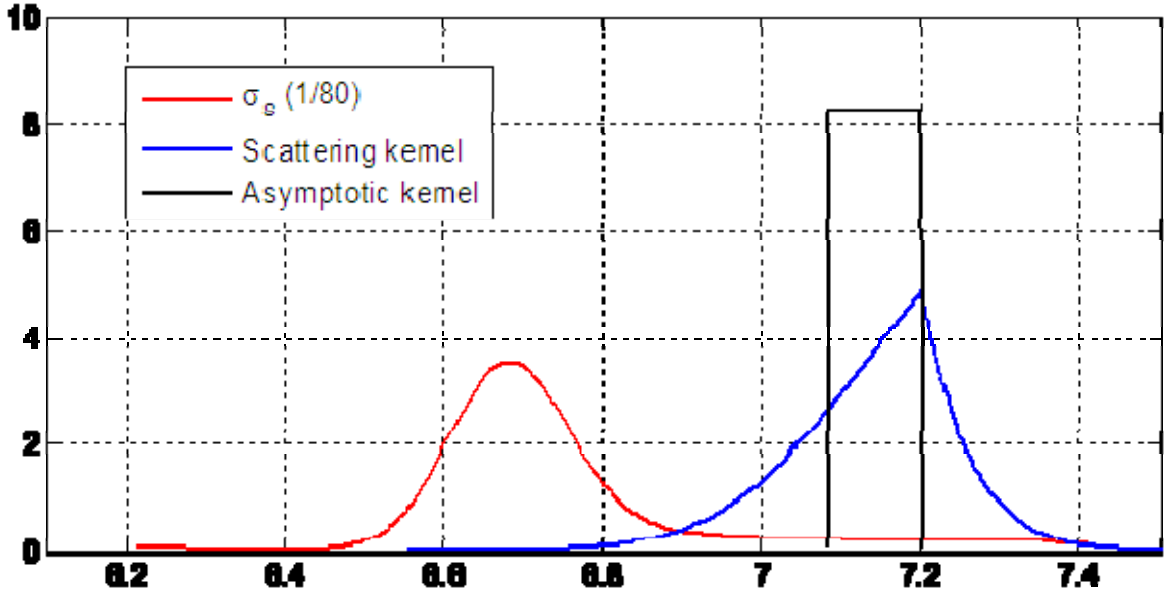
Resonance Scattering Model

Effective transfer kernel of ^{238}U at 1000K near the 6.67 eV resonance or neutrons of energy 6.52 eV



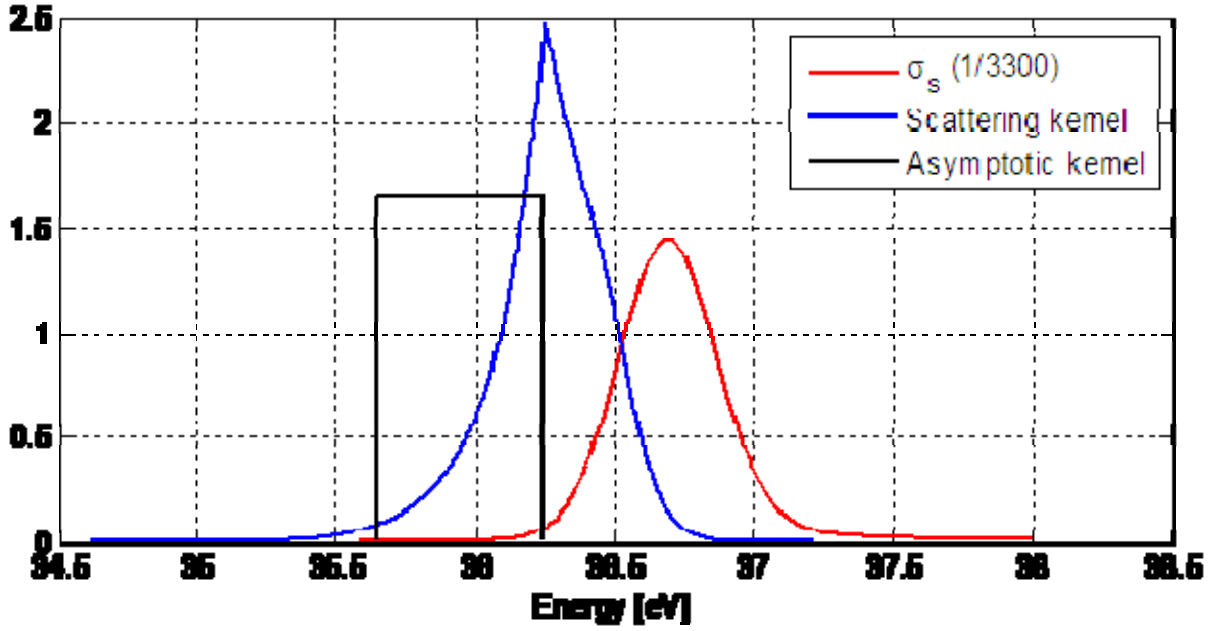
Resonance Scattering Model

Effective transfer kernel of ^{238}U at 1000K near the 6.67 eV resonance or neutrons of energy 7.2 eV.



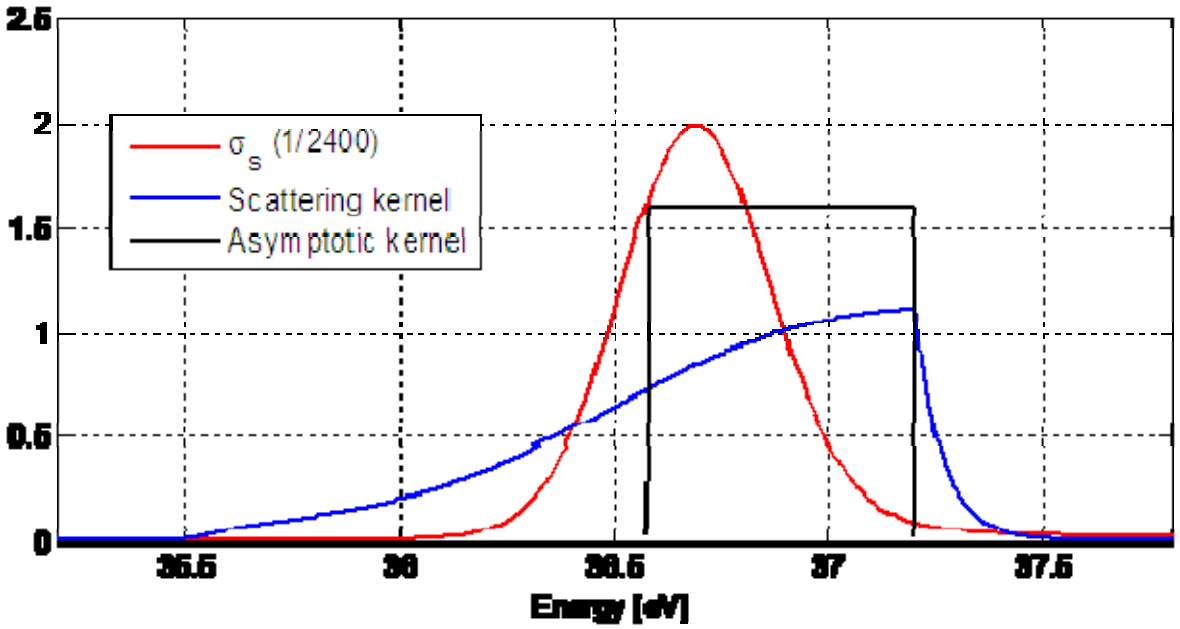
Resonance Scattering Model

Effective transfer kernel of ^{238}U at 1000K near the 36.67 eV resonance or neutrons of energy 36.25 eV.



Resonance Scattering Model

Effective transfer kernel of ^{238}U at 1000K near the 36.67 eV resonance or neutrons of energy 37.2 eV.



Selection of Group Structure

- Examine a new fine group structure (for cross-section generation) optimized for compositions expected in the NGNP
- Well-known multi-group structures exist for different applications
- General Atomic 193-energy group structure (used mostly for prismatic AGCR applications)
- VSOP 98-energy group structure (used mostly for pebble-bed AGCR applications)
- SHEM 281-energy group – developed for UOX and MOX LWR applications
- Refined SHEM 361-group structure

Selection of Group Structure

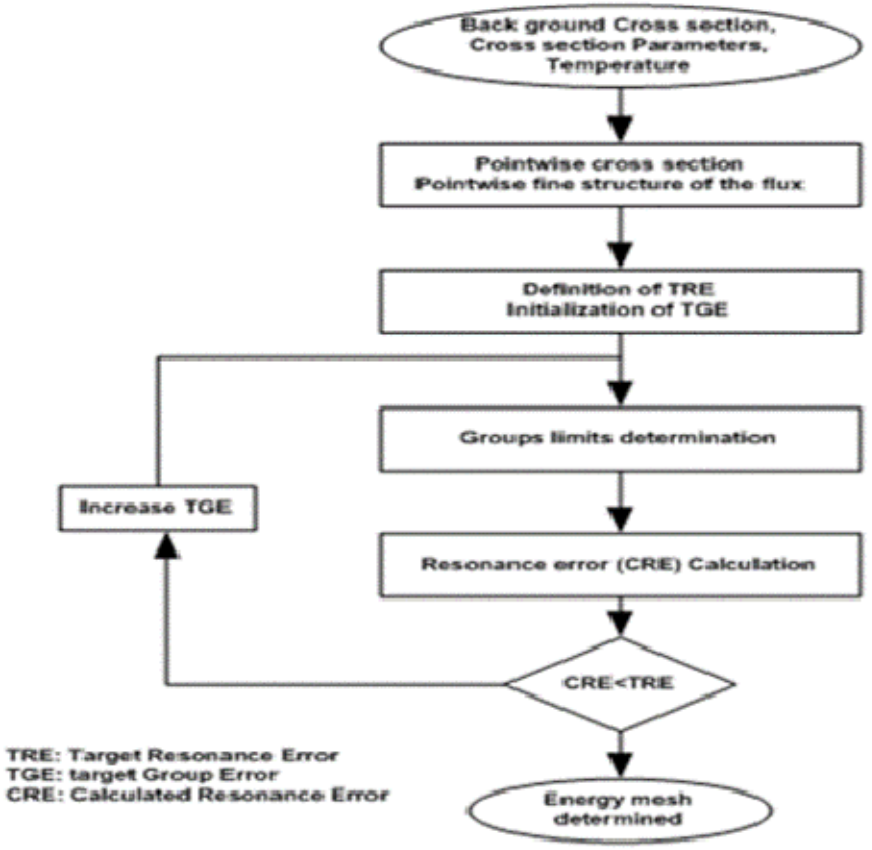
- Comparison and analysis of energy group structures of existing fine group (multi-group) cross-section libraries of spectrum/cell codes utilized for beginning-of-cycle and end-of-cycle studies of prismatic HTR, or for equilibrium core PBR HTR analyses
- New library will be based on the SHEM group structure and subject it to the same sensitivity study
- Considerations that stem from massive presence of graphite, very high burn-up and presence of large inventories of actinides will be included
- SHEM group structure is optimized for light water reactor applications, addressing fuel components as well as structural materials expected to be present

Selection of Energy Structure

The reference fine energy group structure that forms the basis for this study is the SHEM group structure – based on optimization of isolated resonances in different energy ranges in order to avoid the special resonance self-shielding procedures:

- **Thermal energies (0-0.25eV)**
- **Epithermal energies (0.25 - 4eV)**
- **Large resonances (4 -23eV)**
- **Resonances above 23eV**

Selection of Energy Structure



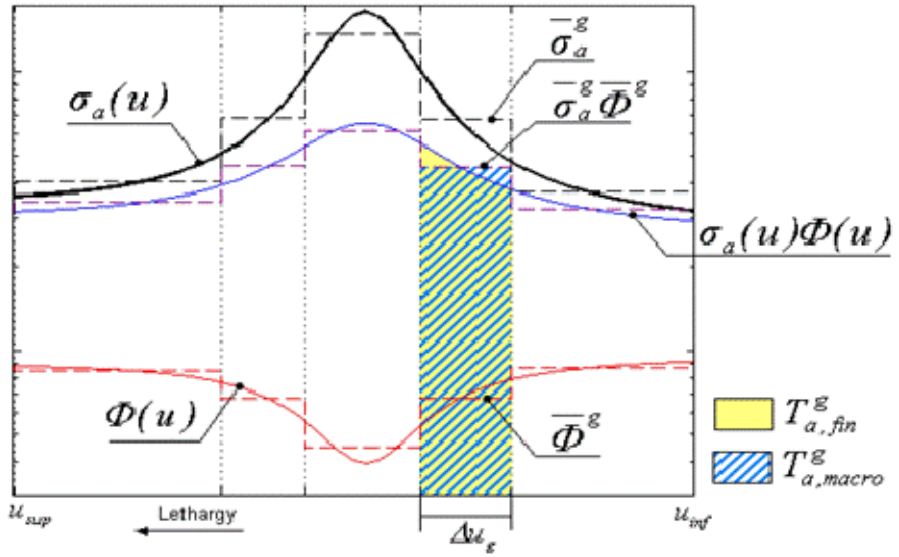
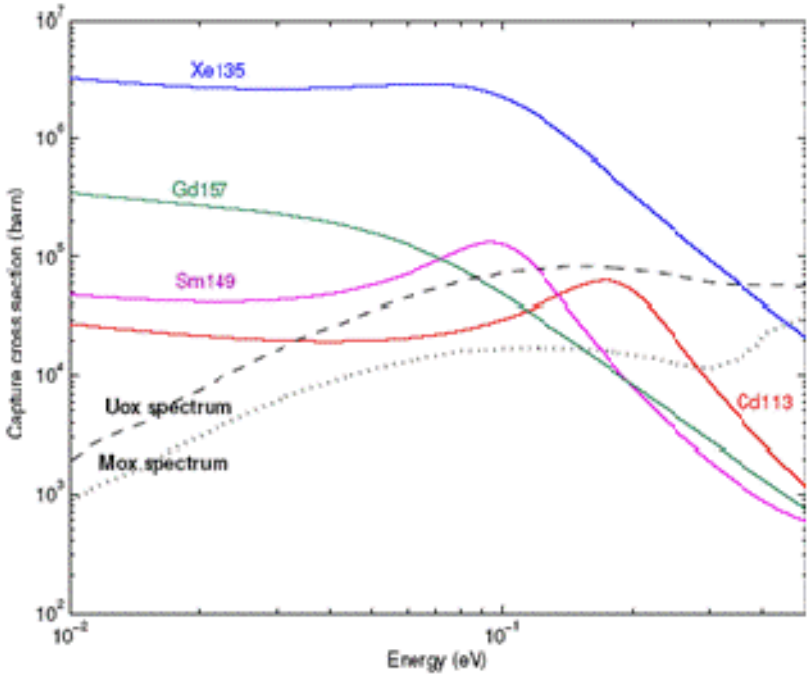


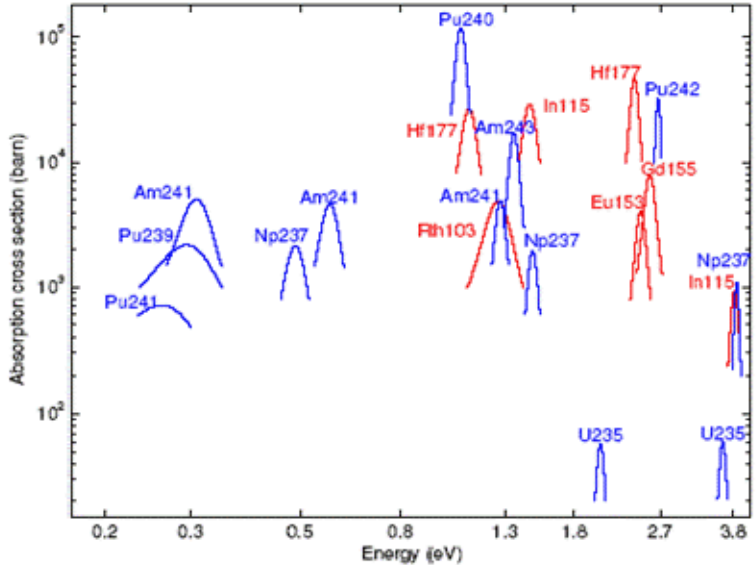
Figure 1. Optimization algorithm for energy mesh inside a resonance

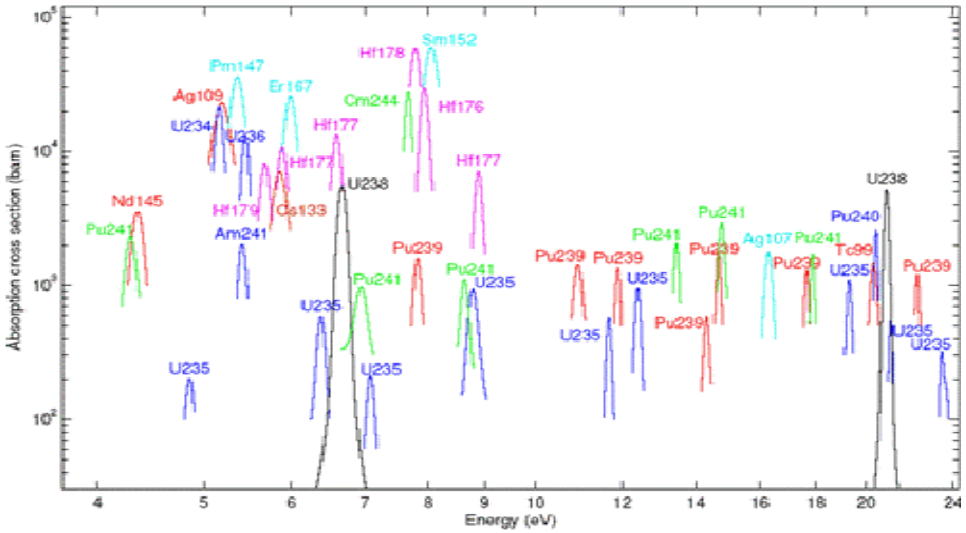
Selection of Energy Structure



Thermal energies (0-0.25EV)

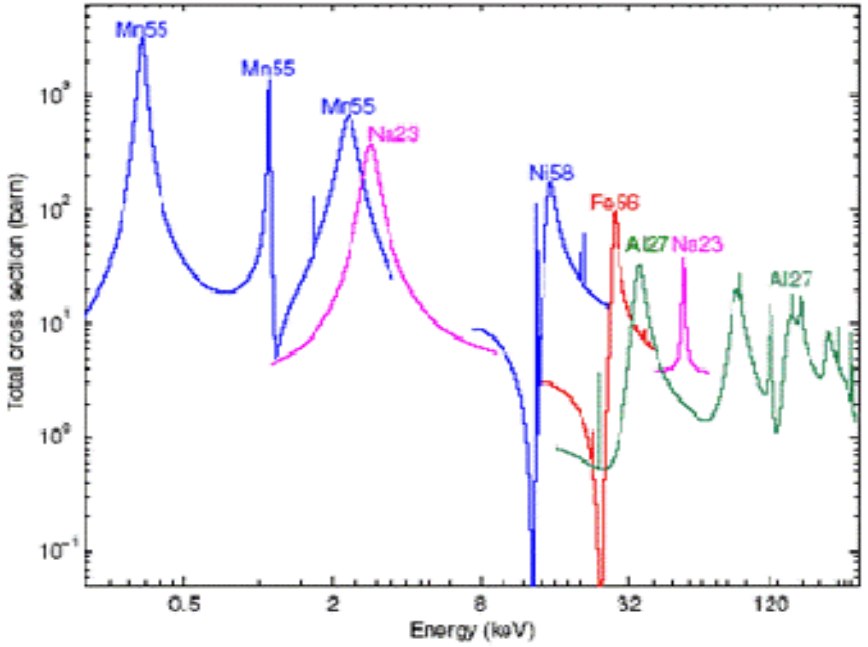
Epithermal energies (0.25-4eV)



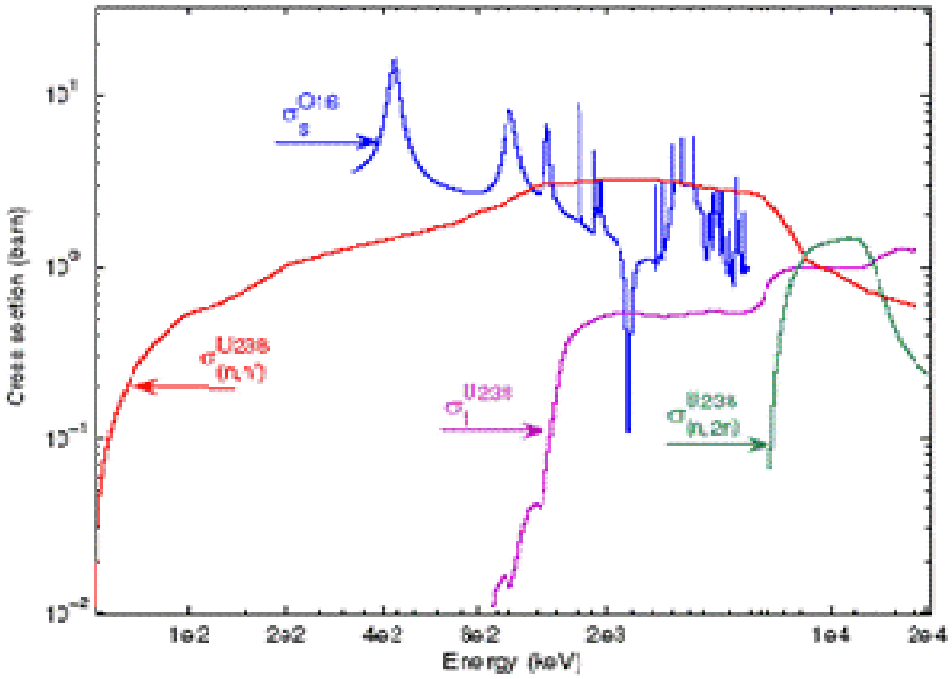


Large resonances (4-23eV)

Selection of Energy Structure



Resonances above 23eV



Selection of Group Structure

- Examine a new fine group structure (for cross-section generation) optimized for compositions expected in the NGNP
- Optimization will be carried out further to produce a finalized coarse-group structure (for core calculations) that takes advantage of the newer fine group structure
- The reference fine energy group structure that forms the basis for this study is the SHEM group structure of Santamarina and Hfaiedh
- Examine the potential shortcoming of SHEM, and if deemed useful and necessary, propose appropriate modifications to the group structure to cover all NGNP and Deep Burn-related physical phenomena

Selection of Group Structure

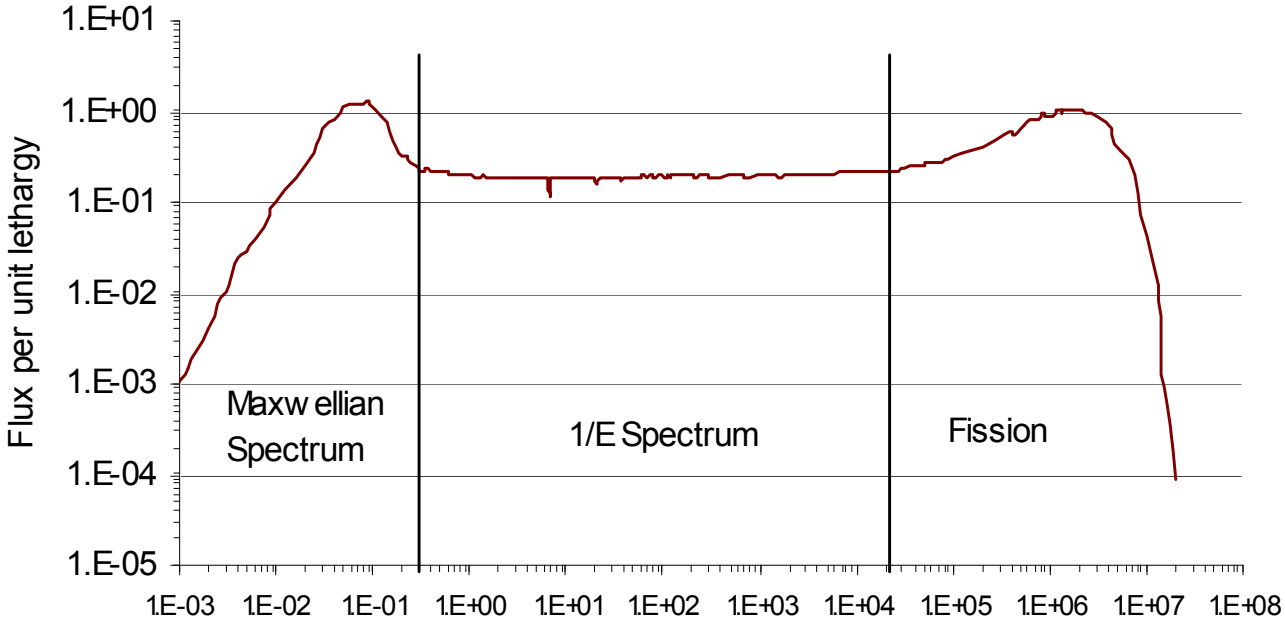
- The SHEM group structure was verified for both Uranium and Mixed Oxide fuels
- In addition, it does address actinides extensively in that resonant reactions are well covered by the structure
- May imply that SHEM structure might be applicable to NGNP and Deep Burn applications without further modification
- Uncertain whether it addresses all actinides that arise in the case of very high burn-up applications, such as those contemplated for NGNP and DB-NGNP
- SHEM structure does not give any particular attention to graphite
- Although the graphite cross sections appear very smooth (with no resonance structures) at all energies below about 2 MeV, the absence of special consideration of graphite may imply an inadequate coverage of the NGNP and Deep Burn physical situations

Selection of Energy Group Structure

- **"Starting" multi-group libraries are being generated using:**
  - Latest version of ENDF/B-VI (ENDF/B-VI.8) and ENDF/B-VII.0
  - NJOY cross-section processing code
  - General Atomic 193-energy group structure, the SHEM 281-energy group structure, and the refined SHEM 369-group structure.
- **Division of these energy group structures into three major ranges of energy: Fast, Epithermal and Thermal**
- **Correlating the group structure to the predominance of selected reactions and reaction rates**
- **Accuracy of multi-group cross-section depends on selected energy group structure and utilized weight function**

Selection of Energy Group Structure

- **Weight function may consists of:**
  - A Maxwellian spectrum (peak at 0.07eV) from 10-5 to 0.3 eV
  - An 1/E spectrum from 0.3 eV to 20.0 keV
  - A fission spectrum from 20.0 keV to 20 MeV



Selection of Energy Group Structure

- **Two target criteria are used for obtaining a fine group structure**
- **First criterion is 10 pcm relative deviation of Δk/k and the second criterion is 1% relative deviation of objective nuclear reaction rates**
- **Objective reaction rates are different for each range of energy:**
  - In terms of reaction and isotope of interest
  - Depending on the most important HTR physical phenomena being modeled in a given energy range

Selection of Energy Group Structure

- **Intent is to find the "best" energy group structure defined as the structure that minimizes the difference between objective functions (power distribution, reactions rates, reactivity prediction …) between multi-group models and MCNP reference continuous energy model**
- **Differences between this "best" group structure and the reference information may meet, exceed or fall short of the target criteria, depending on physics difficulties present in the model problem at hand (or the absence hereof)**
- **Methodology has been proven to work in terms of consistent development of effective cross section fine- and broad- group structures for a given reactor type calculation**
- **Example for TRIGA applications – N. Kriangchaiporn, "Transport Model based on 3-D Cross-Section Generation for TRIGA Core Analysis", Ph.D. Thesis, The Pennsylvania State University, 2006**

Selection of Energy Group Structure

- **The CPXSD Methodology (Contribution and Point-wise Cross-Section Driven)**
- **Used to construct fine- and broad-group structures**
- **Considered two criteria**
  - 1) Importance of groups
  - 2) Point-wise cross sections of an isotope/material of interest
- **Mark L. Williams, "Generalized Contributon Response Theory", Nuclear Science and Engineering, Vol 108, pp. 355-385, 1991**

Selection of Energy Group Structure

- **Contributon Theory and Contributon Equation**

$$C_g = \int_V d^3r \int_{4\pi} d\Omega \Psi_g(\vec{r},\hat{\Omega})\Psi_g^+(\vec{r},\hat{\Omega})$$

- **Used to construct fine- and broad-group structures**

$\psi_g(\vec{r},\hat{\Omega})$ **is the angular flux**

$\psi_g^+(\vec{r},\hat{\Omega})$ **is the adjoint function dependent on position** $\vec{r}$ **and direction** $\vec{\Omega}$ **in group g**

Selection of Energy Group Structure

Fine Group Generation Procedure

1. Select an initial group structure

2. Process the cross sections

3. Calculate the group importance

4. Identify the group that has max. imp.

5. Refine the group that has max. imp.

6. Refine the other groups

7. Generate the cross section library with the new group structure

8. Calculate objectives and compared with the previous library, if not in criterion, repeat step 3 through 8

Selection of Energy Group Structure

Fine to Broad- Group Generation Procedure

1. Select an initial group structure

2. Fine-group cross sections are collapsed to broad-group

3. Calculate the group importance

4. Identify the group that has max. imp.

5. Refine the group that has max. imp.

6. Repeat step 2 through 5 until the criterion is satisfied

Selection of Energy Group Structure

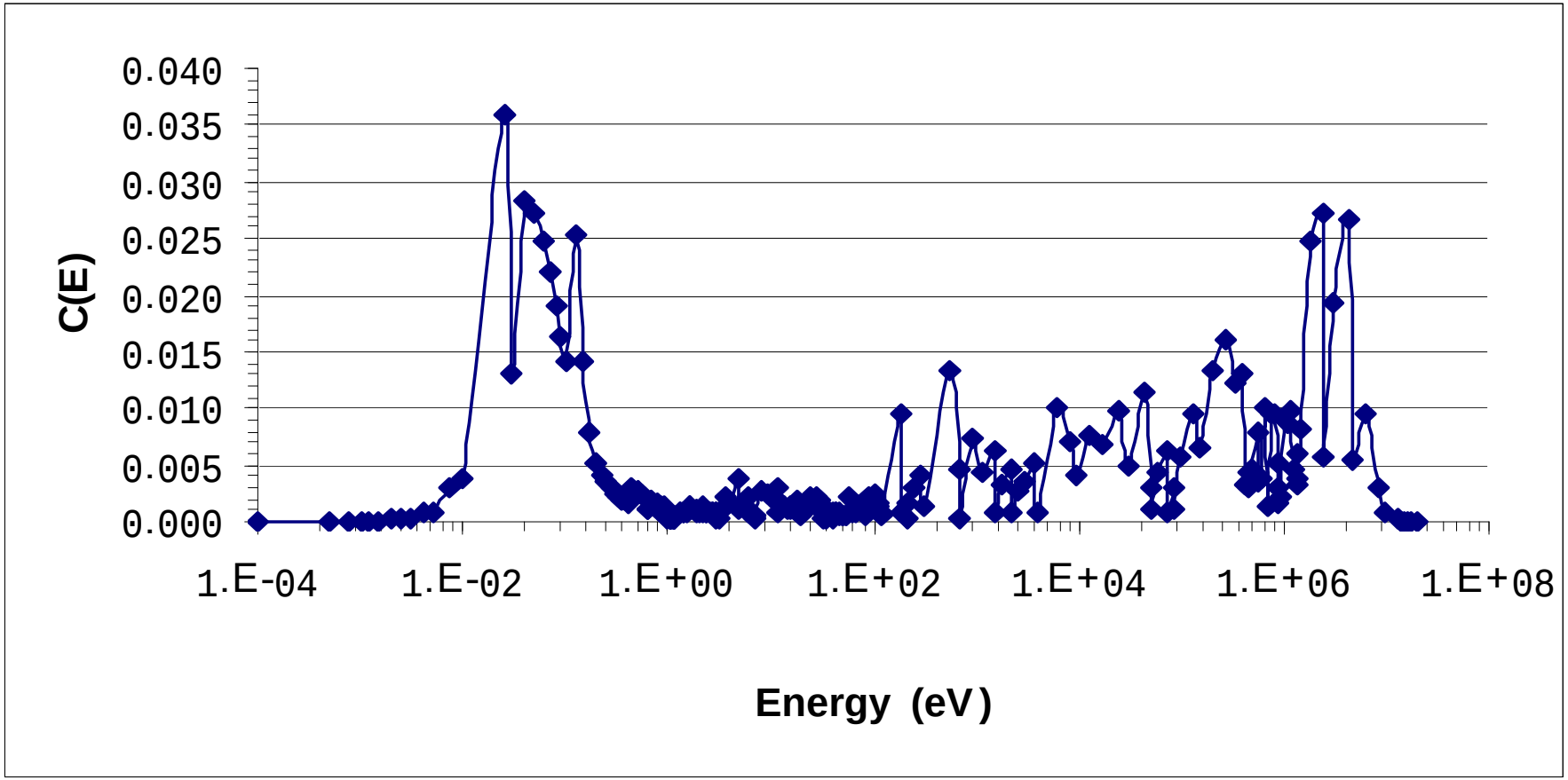
The objective reaction rates:

- Fast energy range: the $^{238}U(n,\nu\Sigma_f)$
- Epithermal energy range: the down-scattering reaction rates of Graphite
- Thermal energy range: the $^{235}U(n,\nu\Sigma_f)$ and the thermal up-scattering reaction rates of Graphite

The criteria for considering fine group structure:

- 10 pcm relative deviation of eigenvalues
- 1% relative deviation of objective reaction rates

Selection of Energy Group Structure



Selection of Energy Group Structure

Weighting Option	*Weighting Strategy*
1.	Flat weighting
2.	Flux weighting
3.	Contributon weighting
4.	Biased importance weighting

$$\sigma_{h,x} = \frac{\sum_{g=h_1}^{h_2} \sigma_{g,x} W_g}{\sum_{g=h_1}^{h_2} W_g}$$

$$\sigma_{l,h' \to h} = \frac{\sum_{g=h_1}^{h_2} \sum_{g'=h_1'}^{h_2'} \sigma_{l,g' \to g} W_g}{\sum_{g'=h_1'}^{h_2'} W_g}$$

1. $W_g = 1$, for a flat "uniform" weighting
2. $W_g = \phi_g$, for a standard flux weighting
3. $W_g = C_g$, for a contributon weighting
4. $W_g = C_g \cdot \phi_g^*$, for *biased* contributon weighting

Selection of Energy Group Structure

- **Software tools (codes) and data (libraries):**
  - The libraries are:
    - ENDF/B-VI.8 (Release 8) and ENDF/B-VII.0 (Release 0)
  - The codes are:
    - NJOY99 nuclear data processing system
    - MCNP Version 5 1.51 and MCOR (Coupled MCNP with KORIGEN)
    - DRAGON Release 4.0.2 and COMBINE-7 lattice physics codes
    - Implementation of the "contributon" method with DRAGON is under way – includes development of additional routines to calculate necessary quantities and to automate optimization process
- **Benchmark problems for the fine–group (cell analysis) optimization**
  - Problem 1 - Unit elementary HTR (NGNP) fuel cell
  - Problem 2 - Extended hyper-cell model will be developed to account for shadowing effects
  - Problem 3 - Locally homogenized cells that avoid the differences caused by different treatments of shadowing by adjacent fuel particles or elements
- **MCNP5 models for these problems to provide continuous energy reference solutions**

Selection of Energy Group Structure

ENDF – B / VI-8.0
ENDF – B / VII.0
} *continouos*

MCNP5

Develop models

- **Pebble (grain, pebble-1D, pebble-3D)**
- **Prismatic**

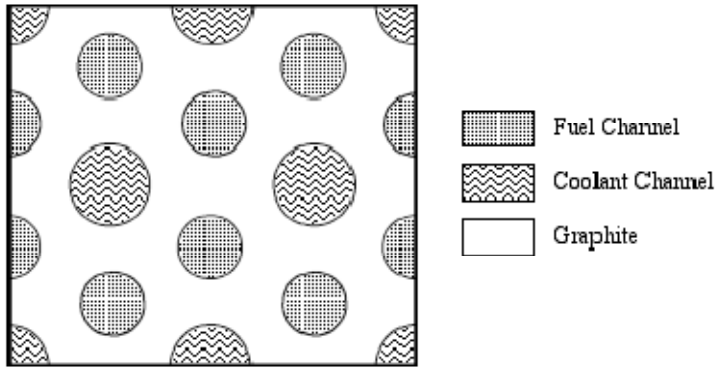
Generate reference solution

NJOY

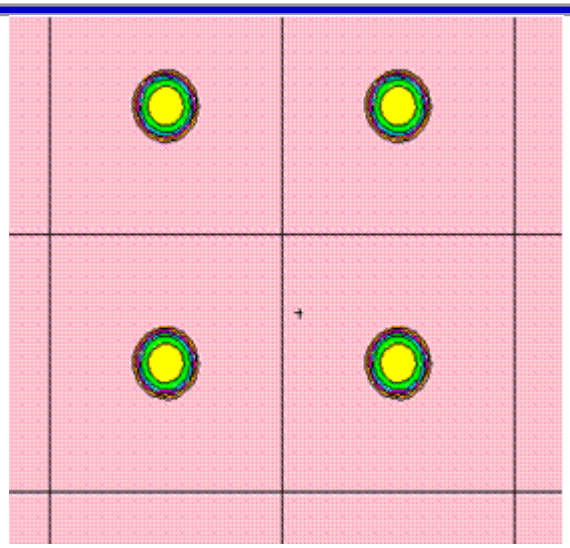
Develop multi-group cross sections (in progress)

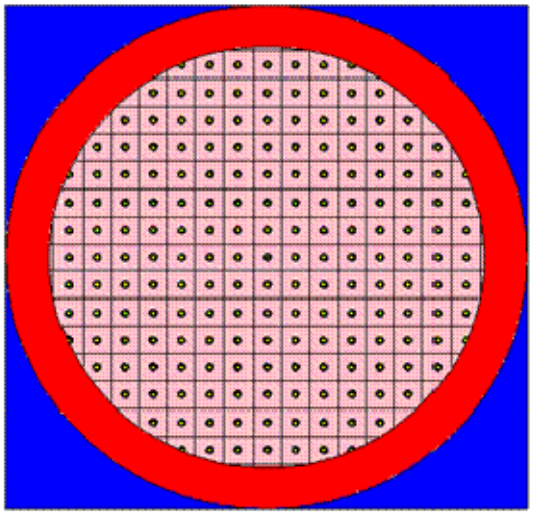
DRAGON

COMBINE

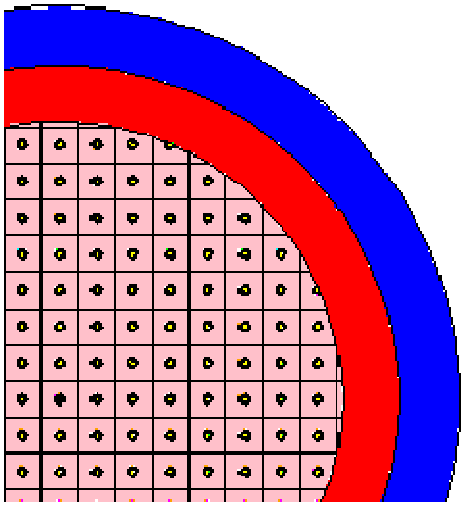


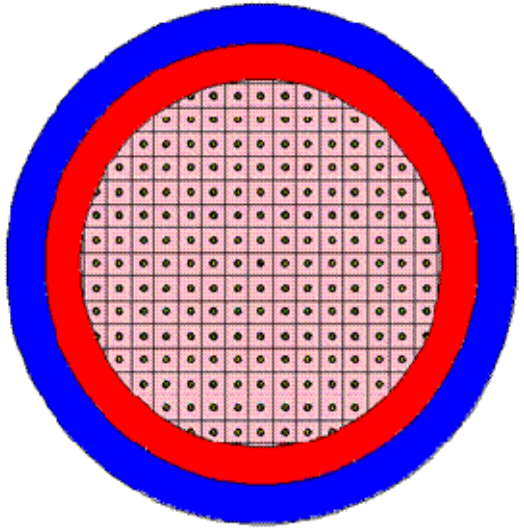
MCNP5 Pebble (Fuel Element) 3D Model



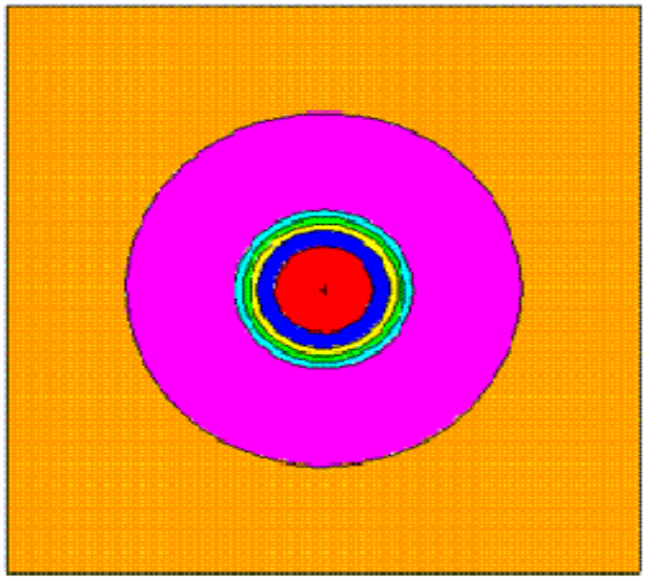


MCNP5 Pebble (Fuel Element) 1D Model

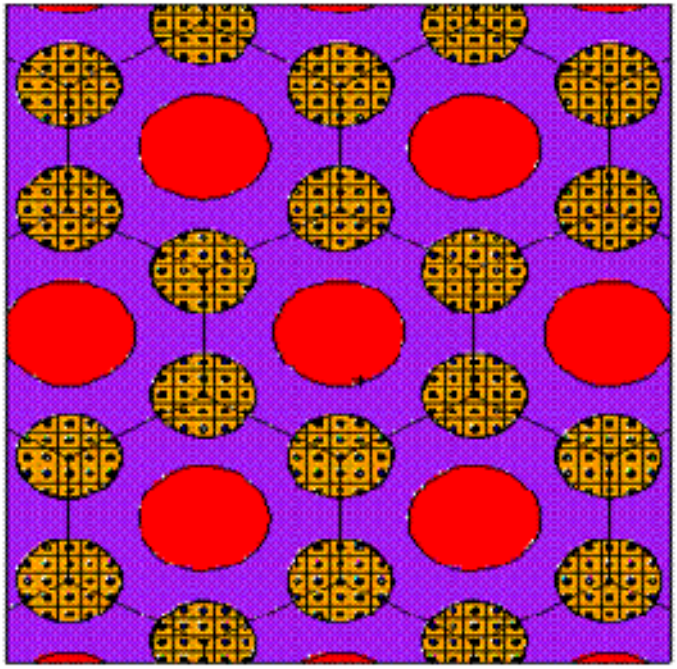




MCNP5 Grain (Coated Particle) Model



MCNP5 Prismatic Lattice Model



MCNP5 Results for Different Models

Model	No Of Histories	Cycles	Keff	Std Dev
CP/Grain	5000	500	1.63054	0.00032
Pebble1D	5000	500	1.53969	0.00026
Pebble3D	5000	500	1.53933	0.00025
Prismatic assembly	5000	500	1.66750	0.00031

Conclusions

- Comparison and analysis of energy group structures of existing fine group (multi-group) cross-section libraries of spectrum/cell codes utilized for beginning-of-cycle and end-of-cycle studies of prismatic HTR, or for equilibrium core PBR HTR analyses
- New library will be based on the SHEM group structure and subject it to the same sensitivity study
- Considerations that stem from massive presence of graphite, very high burn-up and presence of large inventories of actinides will be included
- SHEM group structure is optimized for light water reactor applications, addressing fuel components as well as structural materials expected to be present

Conclusions

- ✓ **Perform a sensitivity study on the broad-group (few-group) energy structure for HTR coupled core steady-state analysis using the CPXSD method utilizing the optimal fine-group libraries**
- ✓ **Outcome will include a new optimized coarse group structure**
- ✓ **Extend the sensitivity study on the broad-group (few-group) energy structure to HTR coupled core transient analysis**
- ✓ **Extend the sensitivity study on the broad-group (few-group) energy structure to HTR Xenon oscillations.**