TRANSPORT CALCULATIONS FOR REACTOR PHYSICS. THE CHALLENGE OF GENERATION IV

BY

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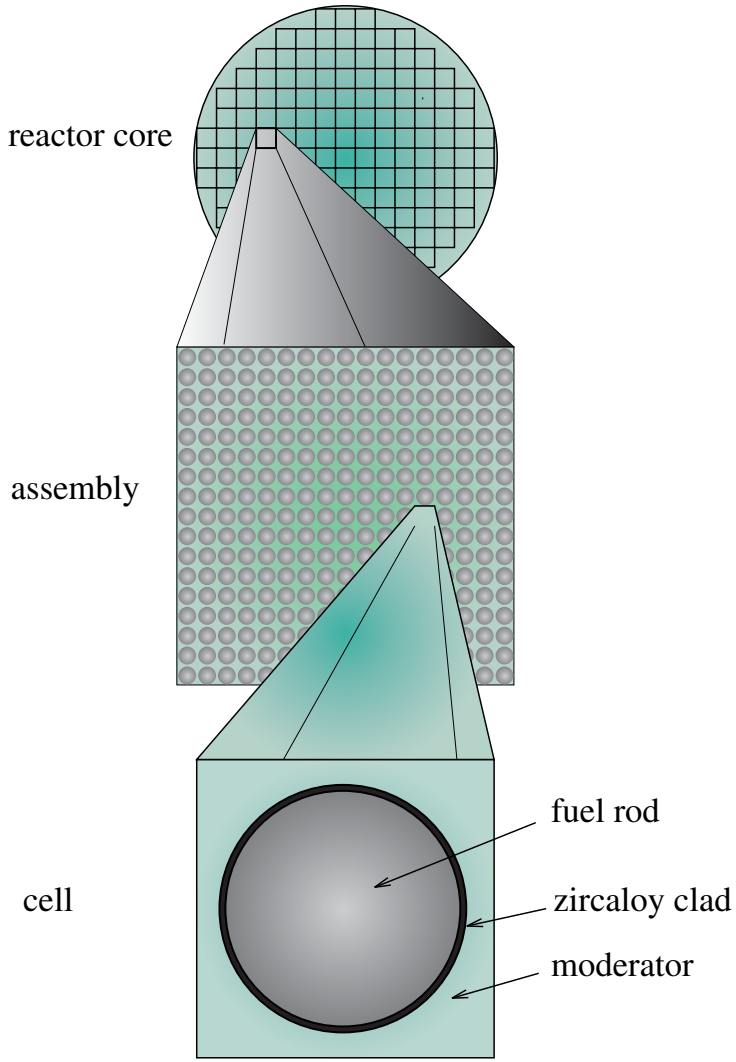
What is a fourth generation Reactor?

- Reactors actually on operation are of 2nd generation.
- Third generation reactors are advanced concepts of 2nd generation ones. Some of them (EPR) are now under construction
- Fourth generation reactors are completely innovative concepts that should be available to the market in 20 or more years.

Classical Homogenization approach



Typical PWR Reactor Geometry

Classical homogeneization theory

If the reactor core has a size ~O(1) and we have to solve mono-energetic the transport problem:

$$(\Omega\nabla+\Sigma)\psi(x,\Omega)=\int_{(4\pi)}d\Omega' f(x,\Omega',\Omega)\psi(x,\Omega')+\lambda\int_{(4\pi)}d\Omega'\Sigma_f(x,\Omega',\Omega)\psi(x,\Omega'),\quad on\ D$$

$$\psi=0\quad on\quad \partial D_-$$

and Xsection are ε-periodic functions, one can write the solution as:

$$\psi(x,\Omega)\sim\psi_0(x,\frac{x}{\varepsilon},\Omega)+\varepsilon\psi_1(x,\frac{x}{\varepsilon},\Omega)+\varepsilon^2\psi_2(x,\frac{x}{\varepsilon},\Omega)+..$$

$$\lambda=\lambda_0+\varepsilon\lambda_1+\varepsilon^2\lambda_2+..$$

where $\psi_i=\psi_i(x,y,\Omega)$ the dependence on x is weak at ε scale, while the dependence on y is fast variating and ε-periodical. One then gets:

$$\psi_0(x,y,\Omega)=u(x)\psi_\infty(y,\Omega)$$

$$\lambda_0=\lambda_\infty,\ \lambda_1=0$$

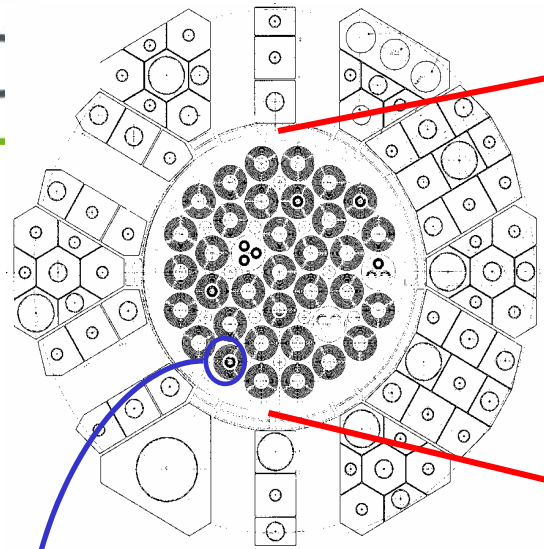
where $\psi_\infty(y,\Omega)$ is the solution of the infinite lattice transport problem, while u:

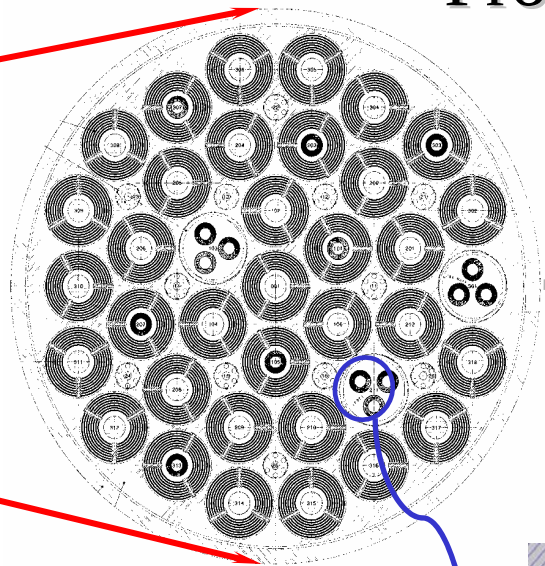
$$-\nabla\overline{\overline{D}}\nabla u=\overline{\sigma}_f u\quad on\quad D,$$

$$u=0\quad on\quad \partial D,$$

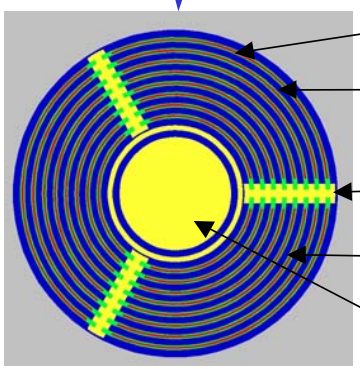
where D and σ are ψ_∞ dependent

Project Calculations : the RJH reactor





Model



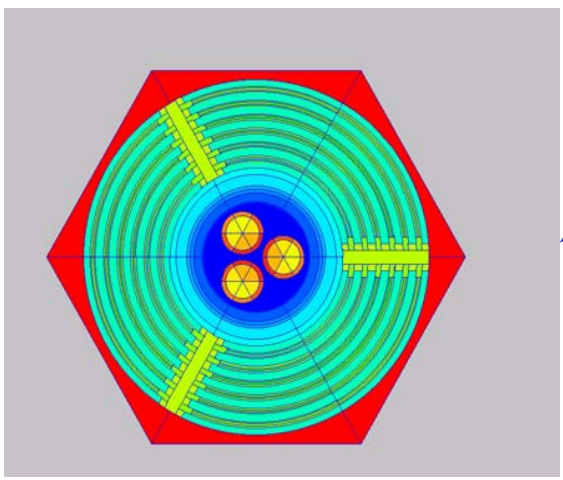
UMoAl
^{235}U 19.75%
thickness 0.61 mm

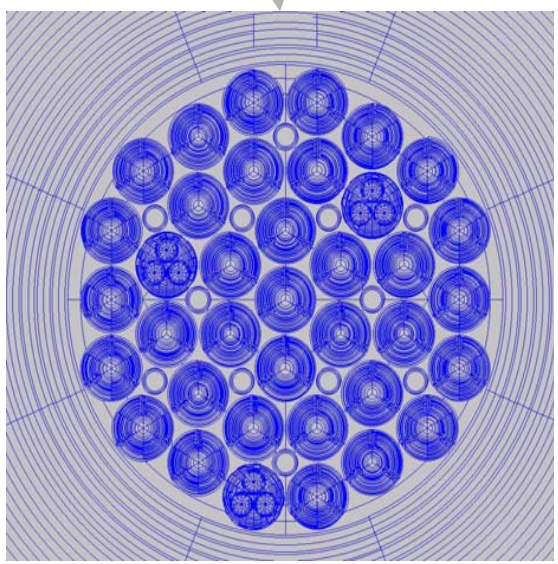
Clad
^{235}U 19.75%
thickness 0.31 mm

stiffener

Water gap
Thickness 0.184

Aluminum filler or
Control rod or
Test device

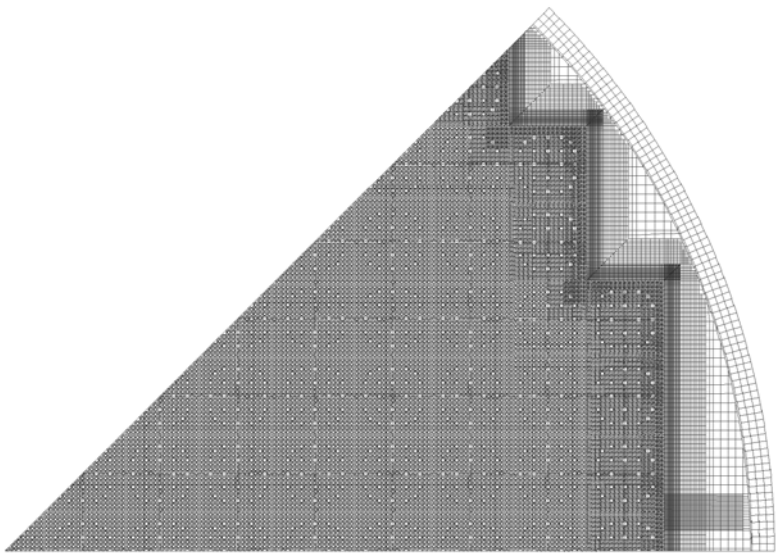




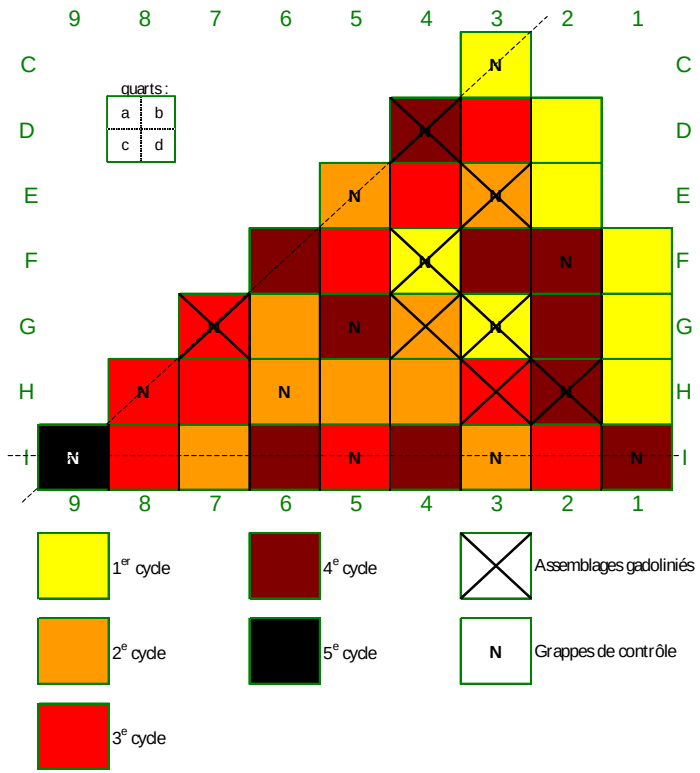
Limits of the classical homogeneization: the EPR case

Third generation Pressurized Water reactor

1/8 EPR computational mesh



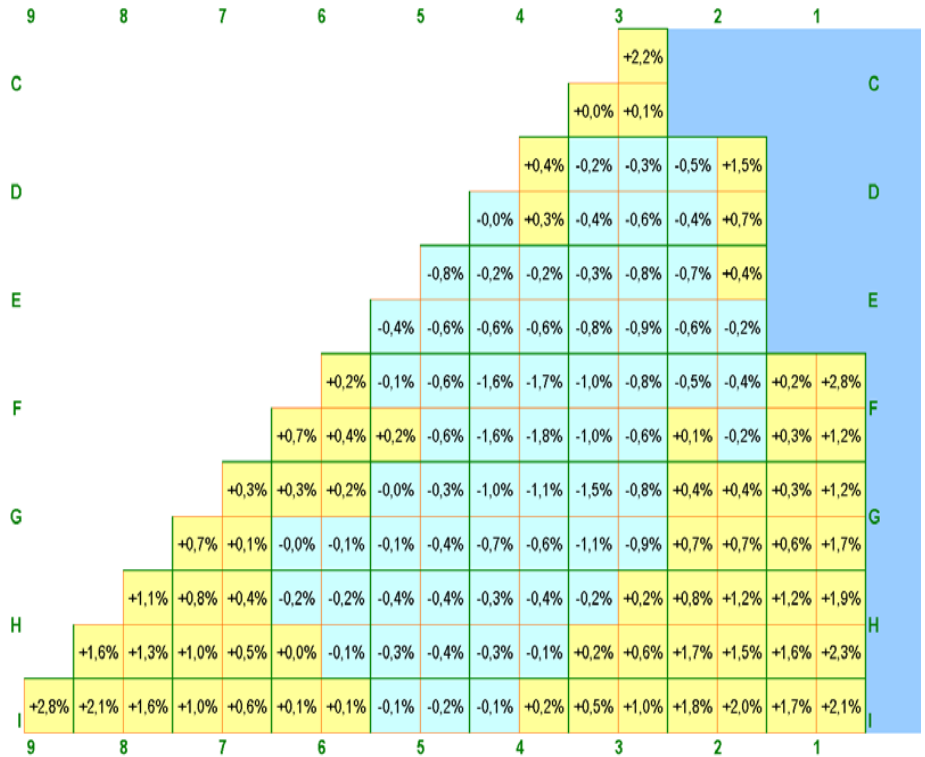
reactor layout: assemblies compositions



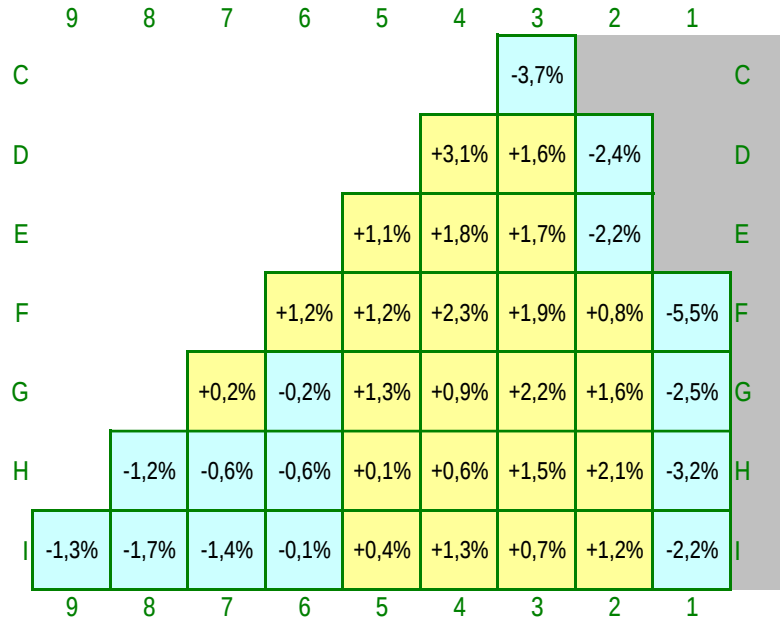
Discrepancies on fission rates

Comparisons done with a reference Montecarlo Calculation

Transport calculation: error on ¼ assemblies



Diffusion calculation: error on assemblies



Even with a not fully converged transport calculation, the interface reactor-reflector errors are strongly reduced

Modern methods for full scale reactors problems: MOC

- *Angular approximation: S_N*
- *Flat flux approximation over homogeneous regions*

$$\psi(\mathbf{r},\Omega) \sim \sum_i \psi_i(\Omega)\theta_i(\mathbf{r})$$

  - *Robust and positive method*
  - *Arbitrary collision anisotropy*

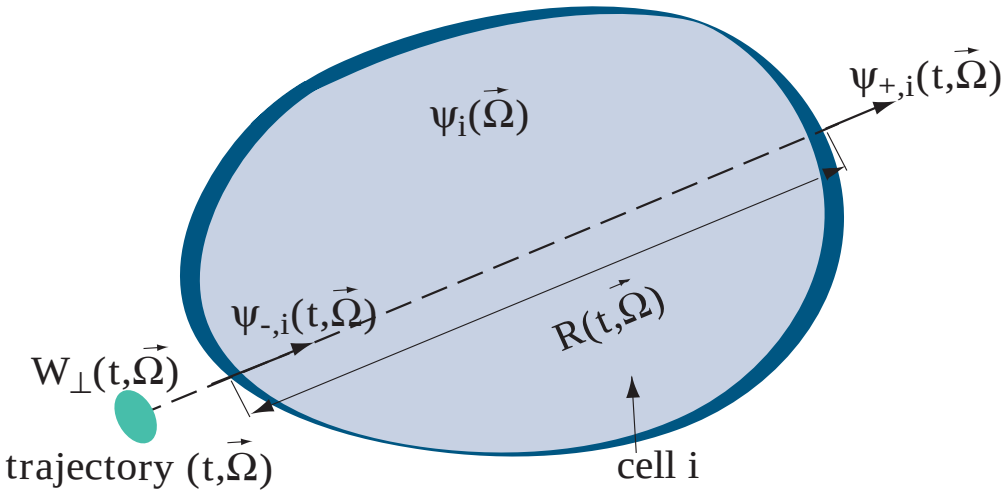
- *iterative solution*

$$\left.\begin{aligned}(\Omega\cdot\nabla+\Sigma)\psi^{(n+1)} &= q^{(n)}\\ \psi_{in}{}^{(n+1)} &= \beta\psi_{out}{}^{(n)}+\psi_0\end{aligned}\right\}$$

$$q^{(n)} = H\psi^{(n)} + S$$

$$albedo\ \ operator\ \beta : \psi_{out} \rightarrow \psi_{in}$$

- *The numerical implementation is based on trajectories*



- *Balance and transmission equation over a trajectory*

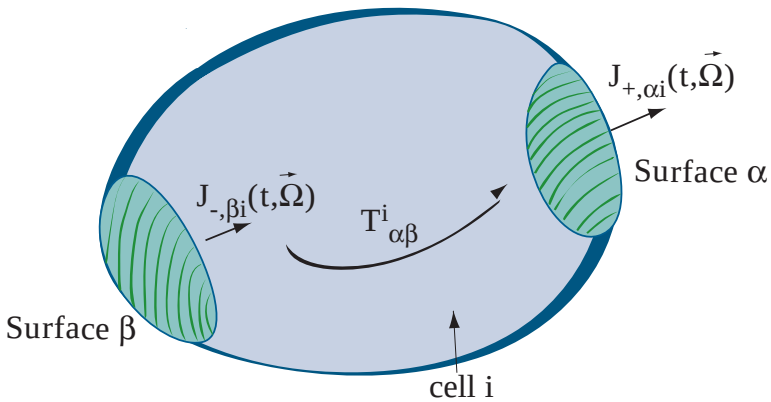
$$\psi_{+,i}^{(n+1)} - \psi_{-,i}^{(n+1)} + \Sigma R\overline{\psi}_i^{(n+1)} = R\overline{q}_i^{(n)}$$

$$\psi_{+,i}^{(n+1)} = T \times \psi_{-,i}^{(n+1)} + E \times \overline{q}_i^{(n)}$$

Synthetic acceleration approach

- *Free iterations :* $B\psi^{(n)} = H\psi^{(n-1)} + S$
- *Problem for the error* $\varepsilon^{(n)} = \psi^{(\infty)} - \psi^{(n)} \rightarrow \left(B - H\right)\varepsilon^{(n)} = H\left(\psi^{(n)} - \psi^{(n-1)}\right)$
- *The transport operator is substituted with a low-order one :*
- *Correct the values of free iterations :* $\psi_{acc}^{(n)} = \psi_{libres}^{(n)} + \delta\tilde{\psi}^{(n)}$
- *Low-order operator : DP_N. It is based on*
  - *Balance equation over a computational region.*
  - *Approximated transmission equation based on surface angular fluxes.*

DP_N Synthetic Acceleration Operator



$$q_i(\mathbf{r},\Omega) \sim \vec{A}_V(\Omega)\cdot\vec{q}_i \qquad \vec{q}_i = \Sigma_s\phi + q_{ext}$$

$$\psi_\pm(\mathbf{r},\Omega) \sim \vec{A}_S(\Omega)\cdot\sum_{\alpha\in\partial i}\vec{\psi}_{\pm,\alpha}\theta_\alpha(\mathbf{r})$$

- *balance & propagation equations :*

$$A^{\rho\upsilon}_\alpha\psi^\upsilon_{+,\alpha} = J^\rho_{\alpha,+} = \sum_{\beta\in\partial i}T^{\rho\upsilon}_{\alpha\beta}\vec{\psi}^\upsilon_{-,\beta} + V_iE_\alpha\vec{q}_i,$$

$$\frac{1}{V_i}\sum_{\alpha\in\partial i}\left(A_\alpha\vec{\psi}_{+,\alpha} - SA_\alpha S\vec{\psi}_{-,\alpha}\right) + \Sigma_i\vec{\Phi}_i = B\vec{q}_i.$$

$$A_\alpha = \iint_{\alpha\times(2\pi)} dSd\mathbf{\Omega}|\mathbf{\Omega}\cdot\mathbf{n}|\,\vec{A}(\mathbf{\Omega})\cdot\vec{A}(\mathbf{\Omega}), \quad S = parity\ of\ \vec{A}(\mathbf{\Omega})$$

- *transmission and escape probabilities (symmetry and conservation preserved by numerical scheme)*

$$T_{\alpha\beta}^{\rho\upsilon} = T_{\beta\alpha}^{\rho\upsilon} = \int_{\alpha} dS \int_{\beta\to\alpha} d\Omega A^{\rho}(\mathbf{\Omega}) A^{\upsilon}(\mathbf{\Omega}) |\mathbf{n}\cdot\mathbf{\Omega}| e^{-\Sigma_i R(\mathbf{r},\mathbf{\Omega})} \quad (symmetry)$$

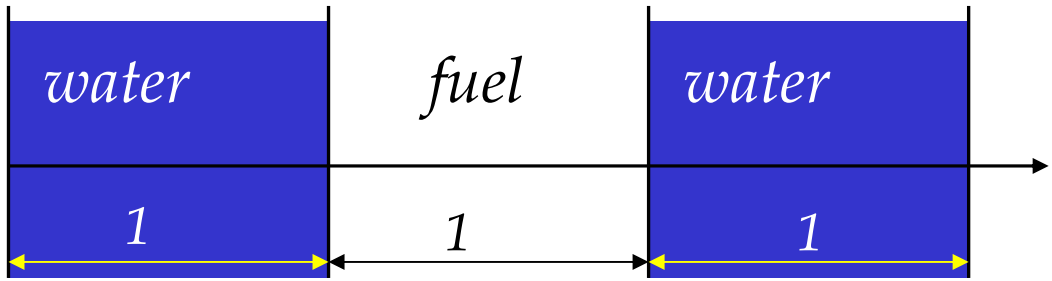
$$E_{\alpha}^{\rho\upsilon} = \frac{1}{\Sigma_i V_i}\left(A_{\alpha}^{\rho\upsilon} - \sum_{\alpha\in\partial i} T_{\alpha\beta}^{\rho\upsilon} \right) \quad (conservation)$$

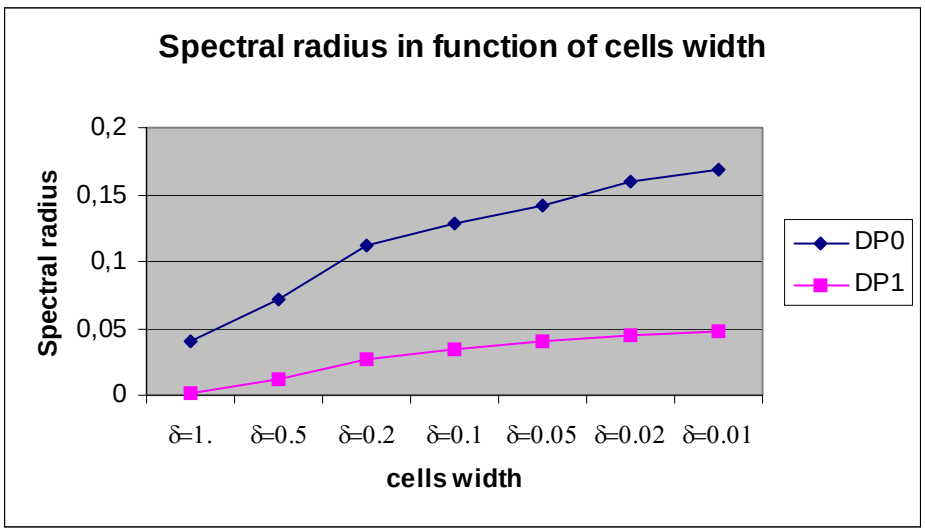
- *numerical evaluation (coherence with transport)*

$$T_{\alpha\beta}^{\rho\upsilon} \sim \sum_{\mathbf{\Omega}} \mathrm{w}_{\mathbf{\Omega}} \mathrm{A}^{\rho}(\mathbf{\Omega}) \mathrm{A}^{\upsilon}(\mathbf{\Omega}) \sum_{(t,\mathbf{\Omega})\in\beta\to\alpha} \mathrm{w}_{\perp}(t,\mathbf{\Omega}) e^{-\Sigma_i R(t,\mathbf{\Omega})}$$

1D Fourier analisys

Benchmark 1D case :





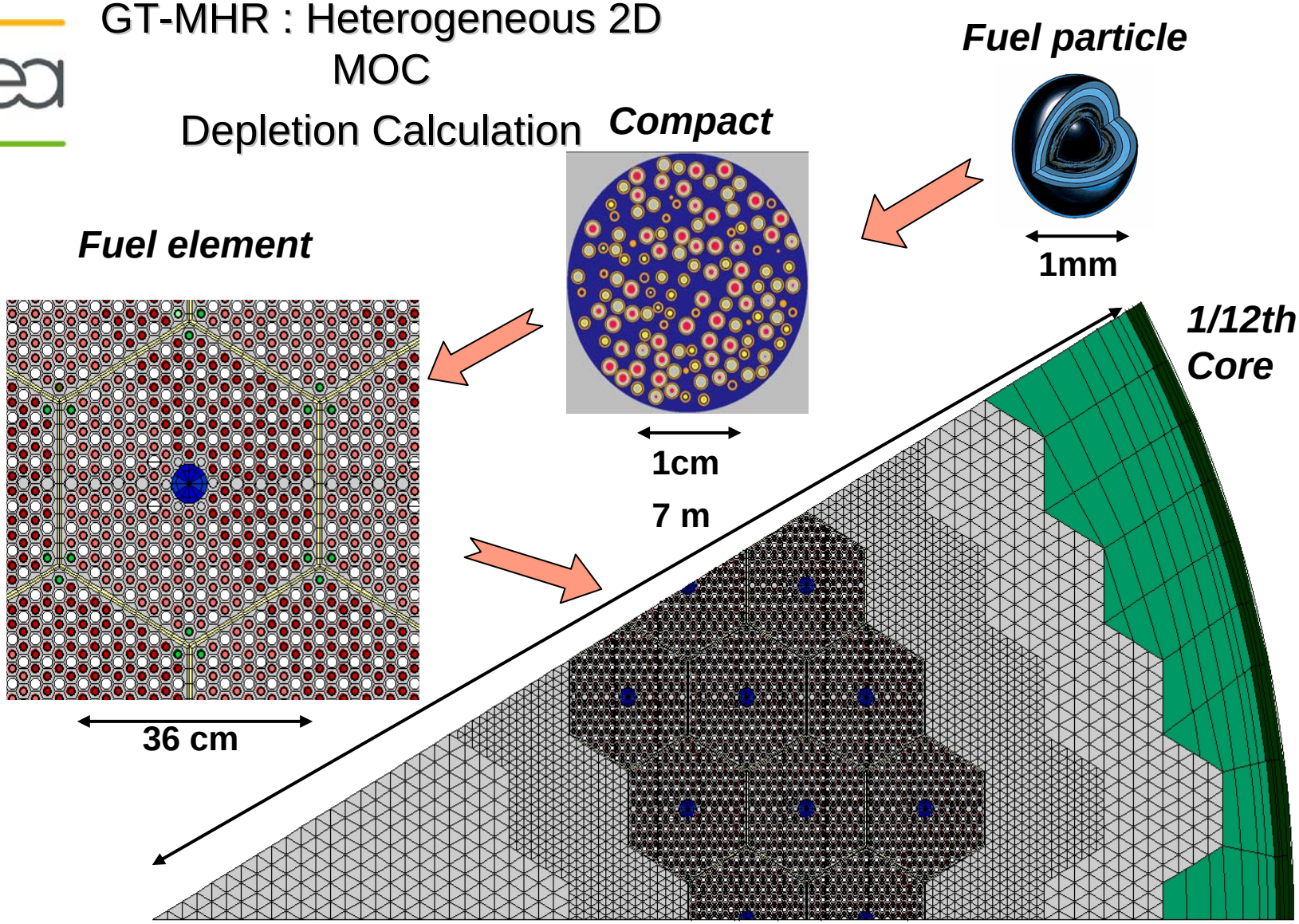
Spectral radius for different integration steps.

- $\rho_{Free} = 0.96$
- $\rho_{DP0} = 0.17$
- $\rho_{DP1} = 0.05$

High Temperature Gas Reactor: the double heterogeneity problem

GT-MHR : Heterogeneous 2D MOC

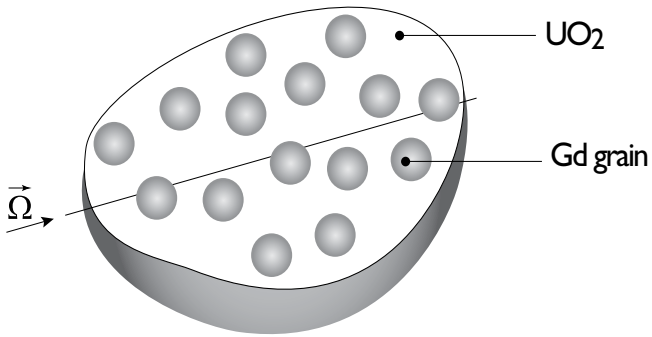
Depletion Calculation



Stochastic media

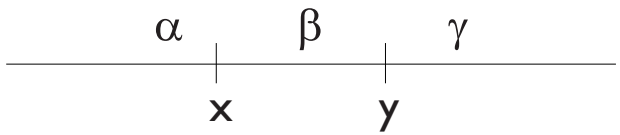
- *Statistical set:* $\Omega = \{\omega, p(\omega)\}$

Realization ω with density of probability p(ω)



- *Multimaterial renewal statistics:*

$$\lim_{|y-x|\to 0} \int_{\Omega_{\alpha\beta\gamma}[x,y]} p(\omega) d\omega = 0$$



- *Homogeneous line statistics*
- *Ensemble average:*

$$x = (\mathbf{r}, \mathbf{\Omega}, E)$$

$$\psi(x) = \int_{\Omega} p(\omega) d\omega \psi_{\omega}(x) = \sum_{\alpha} p_{\alpha}(\mathbf{r}) \psi_{\alpha}(x)$$

Ensemble averaging

- *Material flux:*

$$\psi_\alpha(x) = \int_{\Omega_\alpha(\mathbf{r})} p(\omega) d\omega \psi_\omega(x) \Big/ \int_{\Omega_\alpha(\mathbf{r})} p(\omega) d\omega$$

- $\int$ *equation*

$$(\mathbf{\Omega} \cdot \mathbf{\nabla} + \Sigma_\omega)\psi_\omega = H_\omega \psi_\omega + S_\omega, \quad \omega \in \Omega$$

- *Material averaging operator*

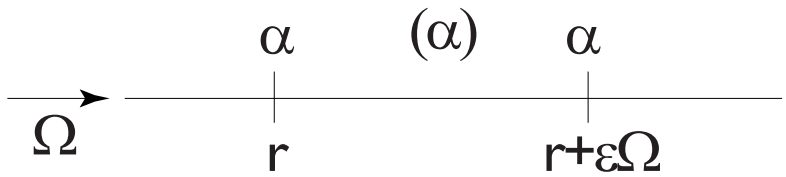
$$[M_\alpha(\mathbf{r})\psi_\omega](x) = \int_{\Omega_\alpha(\mathbf{r})} p(\omega) d\omega \psi_\omega(x)$$

$$M_\alpha(\mathbf{r})\Omega \cdot \nabla \ ?$$

$$\mathbf{\Omega} \cdot \nabla M_\alpha(\mathbf{r})\psi =$$

$$\lim_{\varepsilon \to 0_+} \frac{1}{\varepsilon}[M_\alpha(\mathbf{r} + \varepsilon\mathbf{\Omega})\psi(\mathbf{r} + \varepsilon\mathbf{\Omega},..) - M_\alpha(\mathbf{r})\psi(\mathbf{r},..)]$$

Ensemble averaging



(α)=any material different from α

$$\Omega_\alpha(\mathbf{r}) = \Omega_{\alpha\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega}) \cup \Omega_{\alpha(\alpha)}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega})$$

$$\Omega_\alpha(\mathbf{r}+\varepsilon\mathbf{\Omega}) = \Omega_{\alpha\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega}) \cup \Omega_{(\alpha)\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega})$$

$$M_\alpha(\mathbf{r}+\varepsilon\mathbf{\Omega})\psi(\mathbf{r}+\varepsilon\mathbf{\Omega},..) =$$
$$[M_{\alpha\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega}) + M_{(\alpha)\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega})]\psi(\mathbf{r}+\varepsilon\mathbf{\Omega},..)$$

$$M_\alpha(\mathbf{r})\psi(\mathbf{r},..) =$$
$$[M_{\alpha\alpha}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega}) + M_{\alpha(\alpha)}(\mathbf{r}, \mathbf{r}+\varepsilon\mathbf{\Omega})]\psi(\mathbf{r},..)$$

Ensemble averaging

hence

$$\mathbf{\Omega}\cdot\nabla M_{\alpha}(\mathbf{r}) \equiv M_{\alpha}(\mathbf{r})\mathbf{\Omega}\cdot\nabla + \partial M_{(\alpha)\alpha}(\mathbf{r},\mathbf{\Omega}) - \partial M_{\alpha(\alpha)}(\mathbf{r},\mathbf{\Omega})$$

with

$$[\partial M_{\alpha(\alpha)}(\mathbf{r},\mathbf{\Omega})\psi_{\omega}](x) = \lim_{\varepsilon\to 0_{+}} \frac{1}{\varepsilon}\int_{\Omega_{\alpha(\alpha)}(\mathbf{r},\mathbf{\Omega})} p(\omega)d\omega\psi_{\omega}(x) =$$

$$= \sum_{\beta\neq\alpha} p_{\alpha\beta}(\mathbf{r},\mathbf{\Omega})\psi_{\alpha\beta}(x)$$

Interface flux:

$$\psi_{\alpha\beta}(x) = [\partial M_{\alpha\beta}(\mathbf{r},\mathbf{\Omega})\psi_{\omega}](x)\,/\,[\partial M_{\alpha\beta}(\mathbf{r},\mathbf{\Omega})1](x)$$

Ensemble averaging

- *First balance equation*

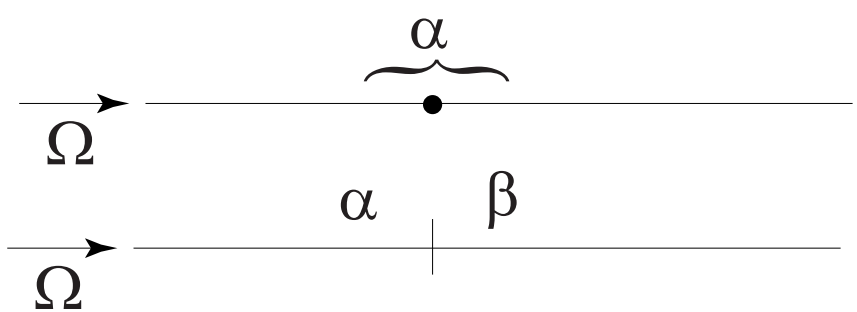
$$(\mathbf{\Omega}\cdot\mathbf{\nabla}+\Sigma_\alpha)p_\alpha\psi_\alpha = p_\alpha(H_\alpha\psi_\alpha + S_\alpha)$$

$$+\sum_{\beta\neq\alpha}(p_{\beta\alpha}\psi_{\beta\alpha} - p_{\alpha\beta}\psi_{\alpha\beta})$$

- *Markovian closure:*

$$\begin{array}{ll} Markovian\ \ statistics & \\ + & \Rightarrow \psi_{\alpha\beta}(x) = \psi_\alpha(x) \\ Collisionless\ \ transport & \end{array}$$

- *Markovian model*



$$(\mathbf{\Omega}\cdot\mathbf{\nabla}+\Sigma_\alpha)p_\alpha\psi_\alpha = p_\alpha(H_\alpha\psi_\alpha + S_\alpha)$$

$$+\frac{1}{\lambda_\alpha(\mathbf{\Omega})}(\sum_{\beta\neq\alpha} t^L_{\beta\alpha}(\mathbf{\Omega})\psi_\beta - \psi_\alpha)$$

Renewal approach 1

transition point = *position at the interface between two materials*

Renewal statistics *'the conditional probability for the material distribution to the right of a transition point is independent of the material distribution to the left': the probability density depends only on what there is at the right of point y*

Renewal equations for material fluxes:

$$\psi_\alpha(x) = R_\alpha(x)e^{-\Sigma_\alpha x}\psi^{in} + \int_0^x e^{-\Sigma_\alpha(x-y)}[R_\alpha(x-y)q_\alpha(y) + g_\alpha(x-y)\psi_\alpha^{in}(y)]dy$$

Interior probabilities for length l of material α

$R_\alpha(l) =$ *probability for length* $\geq l$

$g_\alpha(l) =$ *dens. of prob. for length* $= l$

Renewal approach 2

- $\psi_\alpha^{in}(x) =$ *statistical average of the flux entering material* α *at* x $\quad \psi_\alpha^{in}(x) = \sum_{\beta \neq \alpha} t_{\beta\alpha} \psi_\beta^{out}(x)$
- $t_{\beta\alpha} =$ *conditional transition probability*
- *Interface flux* $\quad \psi_\alpha^{out}(x)$
- *Renewal equations for interface fluxes:*

$$\psi_\alpha^{out}(x) = R_\alpha(x) e^{-\Sigma_\alpha x} \psi^{in} + \int_0^x e^{-\Sigma_\alpha (x-y)} [R_\alpha(x-y) q_\alpha(y) + g_\alpha(x-y) \psi_\alpha^{in}(y)] dy$$

Renewal approach 3

- *Markovian matrix (m) + spherical grains (g)*

$$f_m(l) = \frac{1}{\lambda_m} e^{-l/\lambda_m}$$

- *grains do not collapse*

$$t_{mg} = 1$$

- *renewal, homogeneous, line statistics*

$$f_\alpha(l) \rightarrow R_\alpha(l), g_\alpha(l), \quad t_{gm} = \frac{\lambda_m}{p_m}\frac{p_g}{\lambda_g}$$

- *Isotropic grain chord distribution*

$$f_g(l) = \frac{l}{2R_g^2}, \quad \lambda_g = \frac{4}{3}R_g$$

- *The statistics are completely defined by:*
- p_g *= volumetric proportion of grain of type g*
- R_g *= radius of grain of type g*

Renewal approach 4

Interior analytical solution adapted to the MOC

Interfaces fluxes:

$$\psi_m^{out}(x) = e^{-\Sigma x}\psi^{in} + (1-e^{-\Sigma x})\psi^{as}, \quad x \geq 0,$$

$$\psi_g^{out}(x) = \hat{T}_g e^{-\Sigma x}\psi^{in} + (T_g - \hat{T}_g e^{-\Sigma x})\psi^{as} + \psi_g^{out}, \quad x \geq 2R_g$$

with $$\psi^{as} = \frac{1}{\tilde{\Sigma}}(q_m + \frac{1}{\lambda_m}\sum_g t_{gm}\psi_g^{out}), \qquad \psi_g^{out} = \lambda_g q_g E_g$$

$$\tilde{\Sigma} = \Sigma_m + \frac{1}{\lambda_m}\sum_g t_{gm}(1-T_g), \qquad \Sigma = \Sigma_m + \frac{1}{\lambda_m}\sum_g t_{gm}(1-\hat{T}_g)$$

mean fluxes:

$$\overline{\psi}_0 = \left[q + \left(\psi_- - \psi_+\right)/l\right]/\Sigma,$$

$$\overline{\psi}_g = \hat{E}_g\overline{\psi}_0 + (E_g - \hat{E}_g)\psi^{as} + \psi_g^{out}$$

Comparisons of $k_{effective}$ et of the ratio Production/Absorption inside a representative fuel element

	$k_{effective}$ (variations in pcm)	P/A inside the annular zone (variations in pcm)
TRIPOLI4 Particles described with a regular hexagonal lattice	1,4316 ± 45 pcm	1,5753
TRIPOLI4 Particles distributed stochastically inside the fuel element	1,4312 ± 32 pcm (– 30)	1,5760 (+ 40)
APOLLO2 Transport 99 gr X sections P0 corrected $\Delta r = 5.0*10^{-2}$ / $\Delta N = 12$	1,43037 (– 80)	1,57666 (+ 86)

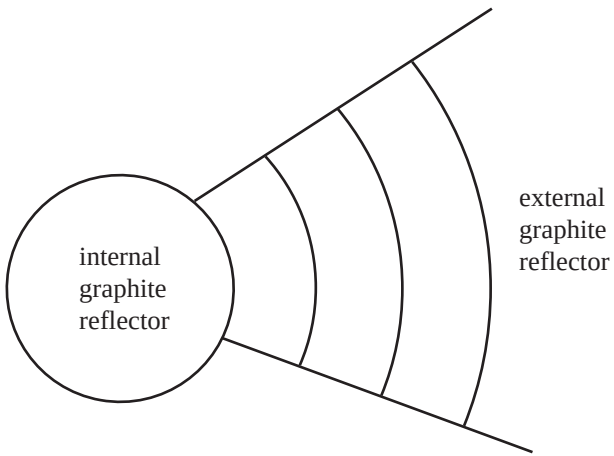
Reactor modelisation in APOLLO2:

- 40000 computational points for the flux calculation
- 35000 s for 1 calculation (99 gr – xsections P0 corrected)

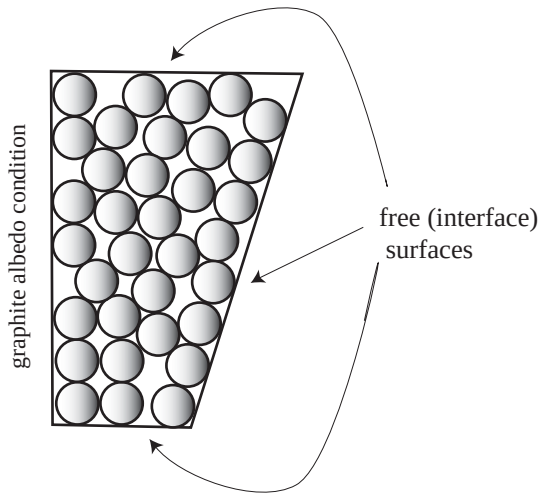
Another scale level: Pebble Bed Reactors (PBR)

PBRs fuel is constituted by pebbles of different types that are stochastically piled up over a cylindrical core. An internal and external circular reflectors delimit the internal and external boundaries for the power region. The cooling is granted by the flow of an Helium gas that pass trough the inter-pebbles space

Horizontal section



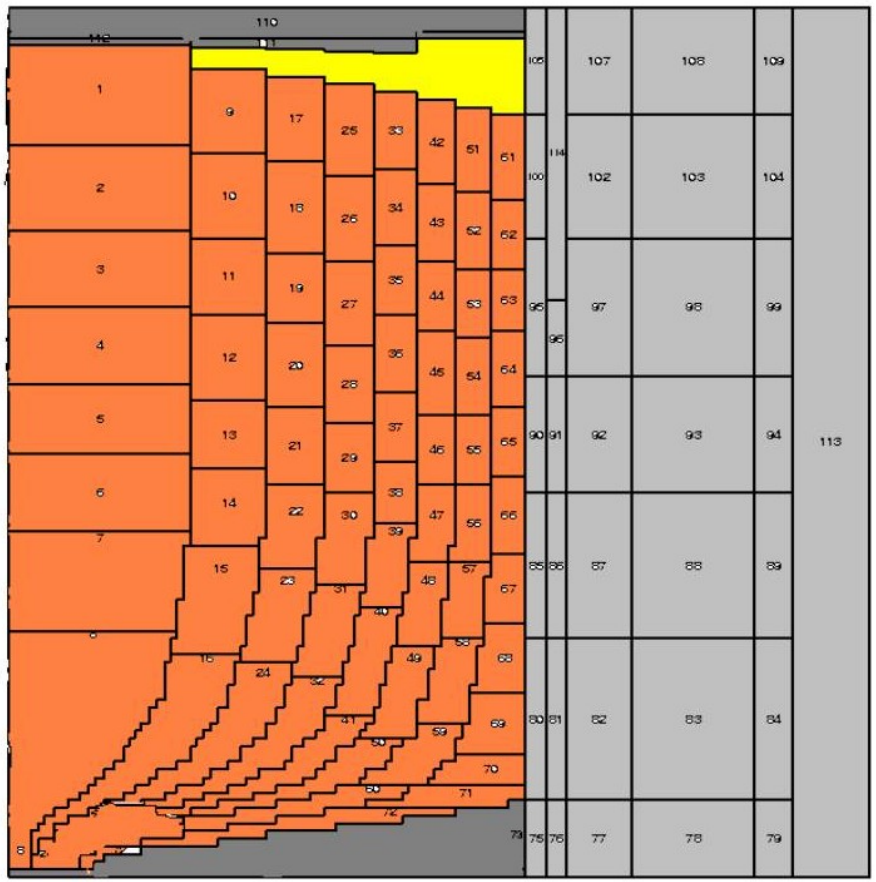
Vertical section



Fuel composition and position are therefore only approximatively known.

PBRs

Several channels exist that drive pebbles toward the lower part of the core where they are progressively discarded. During their path toward the reactor bottom pebbles change their isotope concentration, due to a different burn up.



Numerical techniques for PBRs calculations

- We try to make a diffusion calculation using an engineering equivalence theory. This technique consists in two steps.
- First step: compute an infinite lattice transport solution, used to compute some reference reaction rates.
- Second step: force in the diffusion calculation the conservation of reaction rates of the infinite transport lattice case over macro groups and layers.

$$\Sigma_h^G \Phi_h^G V = \tau^G = \sum_{pebbles} V_{pebbles} \sum_{g \in G} \Sigma_{pebbles}^g \varphi_{pebbles}^g$$

Note that $\Phi_h^G = \Phi_h^G(\Sigma_h^G)$ so that the problem is non linear!

Generally some supplementary constraints are imposed to the equivalence, such as the conservation of the integrated reference flux.

Once a macro flux is obtained from the solution of the diffusion calculation in each layer, the pebble region fluxes are computed from the following factorization:

$$\Phi_{reconstructed,pebbles}^g = \phi_{Diffusion}^G \times \varphi_{pebbles}^g$$

Step 1: infinite lattice calculation

- For each layer we write

$$(\Omega\nabla+\Sigma)\psi = H\psi + \frac{1}{\lambda}P\psi, \quad x \in X$$
$$J_+(E) = J_-(E), \qquad x \in \partial X_-$$

where X is the phase space associated to the layer. Supposing that each pebble occupies every available position with the same probability, and supposing isotropic and uniform entering flux, the problem for pebbles of type “i” is given by:

$$\left(\Omega\nabla+\Sigma_i\right)\psi_i = H_i\psi_i + \frac{1}{\lambda}P_i\psi_i, \quad x \in X_i$$
$$\psi_i = J_-(E)/\pi, \qquad x \in \partial X_{i,-} \qquad \text{(A)}$$

where J_- is the uniform entering current in pebbles. Problem (A) is 1D and can be treated with the CP formalism as

$$\Sigma_{\alpha,i}\phi_{\alpha,i} = \sum_\beta P_{\alpha\beta,i}V_{\beta,i}F_{\beta,i} + I_{\alpha,i}A_iJ_- \qquad \text{(B)}$$
$$A_iJ_{+,i} = \sum_\beta E_{\beta,i}V_{\beta,i}F_{\beta,i} + T_iA_iJ_-$$
$$F = \Sigma_s\phi + Q_{fiss}$$

A relation still remain to be found between entering and exiting currents.

Include the Helium contribution

- To find this last relation we model the inter-pebbles Helium space. The total current of neutrons exiting the spheres and entering other spheres can be written as:

$$AJ_-(E) = \int_S dS \int_{(2\pi)^-} d\Omega |\Omega \cdot n| \langle \psi_- \rangle, \quad A = \sum_i N_i A_i$$

$$\psi_-(r,E,\Omega) = e^{-\Sigma_{He} l} \psi_+(r,E,\Omega) + \int_{[0,l]} dl' e^{-\Sigma_{He}(l-l')} q_{He}(r - l'\Omega, E, \Omega)$$

- Supposing that the source in Helium is uniform and isotropic, as well as the pebble exiting flux one gets

$$\psi_-(r,E,\Omega) = e^{-\Sigma_{He} l} \psi_+(E) + \frac{F_{He}(E)}{4\Sigma_{He}} \left(1 - e^{-\Sigma_{He} l}\right)$$

where *l* is an arbitrary chord length. Making then an average and integrating over surface gives:

$$J_-(E) = \left\langle e^{-\Sigma_{He} l} \right\rangle J_+(E) + \left(1 - \left\langle e^{-\Sigma_{He} l} \right\rangle\right) \frac{F_{He}(E)}{4\Sigma_{He}}, \quad with \quad \left\langle e^{-\Sigma_{He} l} \right\rangle = \int_0^\infty dl p(l) e^{-\Sigma_{He} l}$$

using the markovian distribution $p(l) = \frac{e^{-l/\lambda_{He}}}{\lambda_{He}}$ one gets

$$J_-(E) = \frac{1}{1 + \lambda_{He}\Sigma_{He}} [J_+(E) + \frac{\lambda_{He} F_{He}(E)}{4}] \qquad (C)$$

Final form of the infinite lattice solution

- Add to (B) and (C) a balance equation for Helium

$$\Sigma_{He} V_{He} \phi_{He} = V_{He} F_{He} + A(J_+ - J_-)$$

since

$$J_+ = \frac{\sum_i N_i A_i J_{+,i}(E)}{\sum_i N_i A_i}$$

one has, for a suitable constant C :

$$J_-(E) = C\left(\sum_i N_i \sum_\alpha E_{\alpha i} V_{\alpha i} F_{\alpha i} + E_{He} V_{He} F_{He}\right)$$

that inserted back in (B) gives the final problem to be solved:

$$\Sigma V \vec{\phi} = \tilde{P} V \vec{F}$$

that is an eigenvalue problem for the infinite lattice problem.

Conclusions

- Many challenges are proposed to researchers by innovative 4th generation reactors.
- Strong geometrical heterogeneities prevent traditional homogeneization approaches.
- The presence of stochastic media, both at microscopic and macroscopic level ask to manage with difficult equations.
- More work has to be done…

- For the MOC

Santandrea & Sanchez, Annals of Nuclear Energy, 32,163-193, (2005) (others refs inside)

- For the Double Heterogeneity problem for example

Sanchez & Pomraning, Annals of Nuclear Energy, 18, 371-.., (1991)