RELAP5-3D with PHISICS Neutronics, Part 3 – Depletion Thermo Hydraulic Coupling

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The third newsletter on the RELAP5-3D coupling with PHISICS deal with coupled depletion thermo hydraulic simulation. This is a challenging situation due to the different time scales involved (day/month for the depletion and minutes for the thermo hydraulic).

The Depletion Algorithm

Since the depletion will be a crucial point of this issue, it is worthwhile to consider the types of algorithms PHISICS uses for this task.

The solution of the Bateman depletion burn up equation is essentially the computation of an exponential matrix (given that the flux is assumed constant, thus applying an operator split scheme as in the PHISICS case). The computation of an exponential matrix can be performed in several different ways. Probably the simplest is a Taylor series (one of the code options) but this methodology has the drawback of requiring a very small time step to ensure stability when nuclide decay constants are very small. Using it would force all the other physics into very small size time steps. The Chebyshev Rational Approximation Method (CRMA) has very large stability range, and is therefore the default algorithm. In tests performed, the stability limit was assessed to be equivalent, for a given nuclide, to the time the natural decay would reduce its density of a factor 10^{-7}.

PHISICS performs micro depletion but since it is limited in the number of spatial regions and energy groups, the microscopic cross section should be tabulated as a function of several parameters. The number of parameters and number of points in the tabulation space is unlimited, but a classical set could be: burn-up, xenon concentration, control rod insertion, boron concentration, density moderator, temperature of the fuel (with 3-5 tabulation points each, leading to ~1024 points).

Computer Environment

While depletion is not numerically challenging, even trivial operations can create a large computational burden because of the number of operations by isotopes. This software framework is designed to trace densities of hundreds of isotopes simultaneously in several ten thousand regions. We'll call that $O(10^4)$. Of course, when the depletion is coupled with fuel cycle, cross sections should also be tabulated. That means that an $O(10^3)$ point tabulation should be evaluated for hundreds of isotopes for $O(10^4)$ regions at each time step and a number of exponential matrices, whose size is equal to the number of isotope square $O(10^4)$, should be also computed. It is clear that without a massively parallel approach, this problem could be overwhelming.

PHISICS does, in fact, implement a parallel distribution of the nuclide density that scales the memory demand with the number of processor used for the spatial domain decomposition. Each processor depletes only the spatial domain it sees. This parallel implementation allowed performing the initial validation of this coupling for a PWR startup against experimental data (preliminary result will be presented at the June 2013 ANS).

The coupling scheme

Since no additional modules are added with respect the previous newsletter the different modules are mentioned just to provide enough information to understand the flow chart that follows.

- INSTANT: flux solver (nodal diffusion and spherical harmonics)
- MIXER: parametric interpolation of cross sections, and generation of the macro via density scaling
- MRTAU: depletion burn up solver

The scheme as three iteration indexes:

1. i from 1 to n ranging over time
2. j from 1 to m_i iterative index on the steady state search at each time step
3. k from 1 to N

In the following we have assumed than *dt* is the depletion time step and ΔT is the time step lag between thermo hydraulic updates. The scheme performs n iterations (i index) without updating the thermal hydraulic field, but advancing time. Thereafter, it will stop its time advancement to performed steady state non-linear search (Picard iteration) between neutronics and thermo hydraulic (j index). Once equilibrium is reached, the time iteration restarts for N times (K index)

$$1)\begin{cases} a)\ N^{i+1} = B_m^i\left[\psi^i, N^i\right] \\ b)\ A_m^{i+1} = Tab\left(Th_m, N^{i+1}\right) \\ b)\ F_m^{i+1} = Tab\left(Th_m, N^{i+1}\right) \\ c)\ \psi^{i+1} = \left(A_m^{i+1}\right)^{-1}\left[\dfrac{1}{K_m^{i+1}} F_m^{i+1}\left[\psi^{i+1}\right]\right] \\ d)\ \psi^{i+1} = \psi^{i+1}\dfrac{Power}{\int_V d\vec{r}\,\alpha F_m^{i+1}[\psi^{i+1}]} \\ e)\ B_m^{i+1} = Tab\left(Th_m, N^{i+1}\right) \\ f)\ t \to t + \Delta t \end{cases}$$

if i=n move to system 2

$$2)\begin{cases} P_{j+1}^{i+1}(\vec{r}) = \alpha F_j^{i+1}\left[\psi_{j+1}^{i+1}\right]\dfrac{Power}{\int_V d\vec{r}\,\alpha F_j^{i+1}[\psi^{i+1}]} \\ Th_{j+1}^{i+1} = f\left[P_{j+1}^{i+1}\right] \\ A_{j+1}^{i+1} = Tab\left(Th_{j+1}^{i+1}, N^{i+1}\right) \\ F_{j+1}^{i+1} = Tab\left(Th_{j+1}^{i+1}, N^{i+1}\right) \\ \psi_{j+1}^{i+1} = \left(A_j^{i+1}\right)^{-1}\left[\dfrac{1}{K_{j+1}^{i+1}} F_j^{i+1}\left[\psi_{j+1}^{i+1}\right]\right] \end{cases}$$

Where
N = Nuclide density
ψ = Neutron angular flux
B = Inversion of the Bateman
Tab = tabulation lookup
Th = Thermo-Hydraulic field
F = Fission operator
A = Transport operator
Power = reactor power
α = Energy by fission
f = pseudo steady state inverse of the TH plant model (computed by RELAP5-3D)
N = Nuclide density
B = Inversion of the Bateman equation
Th = Thermo-Hydraulic field
Tab = Table look up

0. Initialization (not showed in the equation sets and in the flow chart)
    a. Simulation starts with a guess in the TH field

   b. Cross sections are generated by the MIXER at the tabulation point
   c. Compute the flux normalized to the provided power

1. The time marching scheme (described in the system 1)
   a. Composition is depleted
   b. The tabulation of the cross section is used to compute the new transport and fission operators
   c. The steady state transport equation is solved for the new fluxes and K_{eff}
   d. Spatial distribution of flux is normalized so that power is match:
   e. Given the new level of burn up the cross section are re-generated
   f. Time advance

If the time is still below the time at which an update of the TH is requested start back from point (1.a) else move to point (2.a)

2. When the TH update time is reached
   a. The normalized power from the last step is computed
   b. RELAP5 3D computes the TH field
   c. Then cross section are updated to account for the change in the TH field
   d. New fluxes and k_{eff} are computed
   e. Loop is restarted from (a) until convergence is reached (Convergence is assumed at j=m)
   f. k=k+1
3. Step 1 and 2 are iterated until the total time reach the end of required depletion and burn up time (k=N)

In the flow chart, the time marching scheme k is not reported since it is beyond the scope of a newsletter article. Essentially the computational flow illustrated in the following picture needs to be repeated N times (k index).

Final Remarks:

Considering that PHISICS allows extreme flexibility in the definition of the cross section, like mixing an arbitrary number of microscopic and macroscopic cross section, the just illustrated schema could be used in a classical approach, where only xenon and other few isotopes are treated explicitly, or where practically all isotopes are treated explicitly. In addition fake isotopes having only decay and production could be also added in an arbitrary number to introduce lumped, neutronically transparent, isotopes to simulate decay heat with an arbitrary number and combination of decay constants. Generally speaking the flexibility in terms of degree of accuracy of RELAP5-3D and PHISICS allow a very detailed sensitivity analysis of the many possible approximation choices. It is in principle possible to use this scheme to simulate one full cycle of the reactor and initiate an accident scenario analysis at any time. Unfortunately the transition from steady state to transient mode for RELAP5 has not yet being automated.

Future work includes the addition of a reshuffling capability that will allow coupled depletion analysis for several years of the life of the reactor.