Coupling of Fuel-Pin and Thermohydraulic Modules in Computer Programs for Reactor Core Analyses

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Abstract

Computer programs dealing with the thermohydraulic analysis of reactor cores (both LWR and LMFBR) usually treat the fuel-pin in a separate module. The reason is that both the fuel-pin and the thermohydraulic phenomena are complicated non-linear problems, and the modules are often developed by differential teams. The advantage of such modularity is that the modules can be updated independently or can be completely replaced. The drawback of modularity is that in fact it is a trend towards explicit algorithms and thereby constraints in time step, in particular when the coupling between the modules is "stiff" in the mathematical sense: high heat transfer coefficients (in LMFBR $\approx 10^3$), two-phase flow, superheat at boiling inception, condensing, reflooding, etc. In safety studies of both LWR and LMFBR these problem areas usually have to be analysed.

This paper deals with a method by means of which a kind of implicit coupling can be implemented between separate modules for fuel-pin and thermohydraulics. The method consists of introducing into the thermohydraulic modules a dummy structure of which the transient behaviour of the nearwall temperature distribution is described accurately during a thermohydraulic time step.
Fuel-pin modules

The heat transport in the fuel-pin is described by a FEM (finite element) or FD (finite difference) discretized equation of the type:

\[ [M] \frac{d[T]}{dt} + [K] \{T\} = \{\phi\} \]  
(1)

\[ [M] = [\rho c R] \] thermal inertia matrix

\[ [K] = \left[ \frac{1}{R} \right] + [h] \] conductivity matrix including gap and film heat transfer

\[ \{T\} \] nodal temperatures

\[ \{\phi\} = \{Q\} + \{hT_m\} \] source term + boundary conditions of medium temperature and film heat/transfer coefficient.

The equations are solved by Galerkin scheme:

\[ \{\Delta T\}^n = [A]^{-1} \left( - [K] \{T\}^n + \{\phi\} \right) \]  
(2)

\[ [A] = \frac{[M]}{\Delta t} + \frac{2[K]}{3} \]

\[ \{T\}^{n+1} = \{T\}^n + \{\Delta T\}^n \]

The allowable time step - from the point of view of accuracy since the scheme is stable - is governed by the response spectrum which depends strongly on the mesh. A fine mesh in the clad would dictate unduly small time steps, as compared to the overall slow response of the fuel-pin (see Appendix 1). In a FEM discretization a single linear element in the clad with nodes at the inner and outer clad wall is sufficient to describe a linear temperature distribution and to evaluate thermal stresses. But even just two nodes in the clad can give rise to time steps which are too small for an efficient use in a reactor core analysis. In such cases subcycling is applied which consists of defining the matrix [A] for a time step which is a fraction of the overall macro time step of the reactor analysis.

\[ \Delta t = Dt/NSUB \]  
(3)

The recurrent relation (2) is then applied NSUB times on an updated RHS, with [A]\^{-1} only triangulated once.

The number of subcycles is defined by the response spectrum of the clad taking into account the high heat transfer coefficient (h \approx 10^5 for LMFBR applications), which is defined by the eigenvalue problem of the clad.

\[ \left[ \begin{array}{cc} -\frac{1}{\tau} & m_{12} \\ m_{21} & m_{22} \end{array} \right] + \left[ \begin{array}{cc} k_{11} & k_{12} \\ k_{21} & k_{22} + h \end{array} \right] = 0 \]  
(4)

The allowable time step for a given eigenvalue \( \tau \) is defined by considering the system with one degree of freedom

\[ \frac{dy}{dt} + \frac{1}{\tau} y = \frac{1}{\tau} y_0 \]  
(5)

The Galerkin numerical solution of (5), similar to (2), can be written as:

\[ \left( \frac{1}{\Delta t} + \frac{2}{3\tau} \right) \Delta y = -\frac{1}{\tau} (y - y_0) \]  
(6)

From (6) it is seen that for \( \Delta t > \tau \) a 50% overshoot is obtained numerically. The exact numerical solution is obtained for \( \Delta t = 3\tau \). The number of subcycles NSUB is defined from the smallest eigenvalue \( \tau \) of (4):

\[ \text{NSUB} = \text{Dt/3} \tau \]  
(7)

and next by (3) the \( \Delta t \) to be used in [A] is defined. The subcycling is limited to NSUB \approx 6. The reason is the unconditional stability of the Galerkin scheme (2) and (6). The maximum overshoot for time steps \( \Delta t > \tau \) is 50%.

In a next cycle the undershoot becomes 25% etc., and with a maximum number of subcycles NSUB \approx 6 the precision becomes \( 2^{-6} = 1.6\% \).
Coupling of pin-fuel and thermohydraulics

The explicit coupling of the fuel-pin to the thermohydraulics consists of applying boundary conditions of extrapolated heat transfer coefficient \( h \) and medium temperature \( T_{m} \) in the fuel-pin module. The fuel-pin module defines the flux to the coolant which is transferred to the thermohydraulic module, where the medium temperature and heat transfer coefficient are updated. There are also other schemes where the thermohydraulics are dealt with first, using an extrapolated clad temperature. The flux is then transferred to the fuel-pin module which updates the clad temperature.

In the explicit methods the immediate feedback of fast changing thermohydraulic conditions is not accounted for. When the flux is extrapolated it remains as it is, despite the fact that the heat transfer coefficient \( h \) or medium temperature \( T_{m} \) changes. When the clad temperature is extrapolated it remains as it is, despite the fact that the response of the wall temperature is rather fast. In the method proposed in this paper the nearly immediate response of clad wall temperature and thereby flux is described by an equation of the type:

\[
\Delta T_{c} = \alpha \cdot \beta \Delta q_{c} \tag{8}
\]

\( \Delta T_{c} \) - variation of clad outer wall temperature in time step \( t \), \( t+\Delta t \) of the thermohydraulic module \( T_{c}^{n+1} = T_{c}^{n} + \Delta T_{c} \)

\( \Delta q_{c} \) - variation of flux to coolant in the time step \( t \), \( t+\Delta t \) (\( q_{c}^{n+1} = q_{c}^{n} + \Delta q_{c} \))

\( \alpha, \beta \) - parameters depending on the current conditions and on the time step \( t \), \( t+\Delta t \) (\( \beta > 0 \))

Equation (8) can be used in various ways depending on how the thermohydraulic module is organized. As an example, for single phase flow the energy equation is usually written in terms of medium temperature \( T_{m} \):

\[
\rho c_{v} \frac{\partial T_{m}}{\partial t} + \rho c_{v} \frac{\partial T_{m}}{\partial z} = h (T_{c}^{n} - T_{m}^{n}) \tag{9}
\]

In discretized form (9) can be written as

\[
A^{n} T_{m}^{n+1} + B^{n} T_{c}^{n+1} = C^{n} \tag{10}
\]

where \( A^{n}, B^{n} \) and \( C^{n} \) are known at time \( t = t^{n} \).

Equation (8) can be written as:

\[
T_{c}^{n+1} = T_{c}^{n} - h^{n} (T_{c}^{n} - T_{m}^{n}) - \Delta q_{c}^{n} \tag{11}
\]

or

\[
-\beta h^{n+1} T_{m}^{n+1} + (1 + \beta h^{n+1}) T_{c}^{n+1} = T_{c}^{n} + \alpha \Delta q_{c}^{n} \tag{12}
\]

Equations (10) and (12) represent an implicit scheme (except for \( h^{n+1} \)) to update \( T_{c} \) and \( T_{m} \).

For two-phase flow, or in general when the main variable is not the medium temperature but rather the enthalpy, eq.(11) should be used within an iteration loop taking care that any possible implicitness is employed to accelerate the convergence. To illustrate it, \( T_{c}^{n+1} \) is written explicitly from (12):

\[
T_{c}^{n+1} = \frac{T_{c}^{n} + \alpha \Delta q_{c}^{n} + \beta h^{n+1} T_{m}^{n+1}}{(1 + \beta h^{n+1})} \tag{13}
\]

The power to coolant at time \( n+1 \) is given by:

\[
\Delta q_{c}^{n+1} = h^{n+1} (T_{c}^{n+1} - T_{m}^{n+1}) \tag{14}
\]

From (13) and (14) one can eliminate \( T_{c}^{n+1} \)
\[ q_{c}^{n+1} = \frac{h^{n+1}(T_{c}^{n} + \alpha + \beta q_{c}^{n} - T_{m}^{n+1})}{1 + \beta h^{n+1}} \]  

(15)

In (15) \( q_{c}^{n+1} \) represents the power to coolant at the end of the time step. A predictor-corrector algorithm is applied by calculating \( T_{m}^{n+1} \) and \( h^{n+1} \) for \( q_{c}^{n} \) or an extrapolated value, etc.

**Transient behaviour of clad wall**

The determination of the parameters \( \alpha \) and \( \beta \) is not carried out in the fuel-pin module; the mesh in the clad is too coarse for an accurate determination. Moreover, the parameters \( \alpha \) and \( \beta \) have to be updated when the thermohydraulic module applies subcycling, i.e. several micro time steps to cover the fuel-pin time step. Indeed modularity gives the possibility of running the modules with different time steps.) To define the current \( \alpha \) and \( \beta \) a dummy structure is introduced in the hydrodynamic modules consisting of a slab of thickness \( d \) (Fig. 1).

![Fig. 1 - Model to simulate skin effect in clads.](image)

The flux defined in the fuel-pin module \( (q) \) is not given to the coolant directly. Instead it is considered as a surface flux into the slab. The slab in turn is cooled by the medium \( (q_{c}) \). A positive or negative mismatch between \( q \) and \( q_{c} \) heats up the slab or cools it down, respectively. The quantity \( (q-q_{c}) \) would be lost for the system since the slab is a dummy structure. For that reason the same quantity \( (q-q_{c}) \) is applied once more as a distributed source, and the overall long-term heat balance is therefore satisfied.

The governing equation of this problem is:

\[
\rho c \frac{\partial T}{\partial t} - \lambda \frac{\partial^2 T}{\partial x^2} = (q - q_{c})/d
\]

BC \( x = 0 \): \(-\lambda \frac{\partial T}{\partial x} = + (q - q_{c}) \) \quad \quad \quad x = d: \quad -\lambda \frac{\partial T}{\partial x} = 0

A FEM discretization is carried out to solve (15) with special attention to the skin effect. To this end the slab is not divided into elements but only one node (at \( x = 0 \)) with several nodal parameters (degrees of freedom DOF) is introduced (Fig. 1):

\[
T = [P_{1}, P_{2}, P_{3}, ...] [T_{1}, T_{2}, T_{3}, ...]^T
\]

\[
P_{i} = (1 - \xi)\xi^{i-1}, \quad \xi = \frac{x}{d}
\]

The classical Galerkin weak formulation of (15) gives the discretized FEM equations:

\[
\rho c d [M] \frac{dT}{dt} + \frac{\lambda}{d} [K] (T) = (q - q_{c}) \{ b \}
\]

\[
m_{d} = \int_{0}^{d} P_{i} P_{j} d\xi
\]
\[
    k_{ij} = \int_0^1 \frac{dP_i}{d\xi} \frac{dP_j}{d\xi} \, d\xi
\]
\[
    b_i = P_i(\xi = 0) + \int_0^1 P_i d\xi
\]
(see Appendix 2 for numerical values.)

The choice of the number of DOF to be taken into account and of the slab thickness \(d\), depends on the response spectrum as compared to the time step in the hydrodynamic analysis. For a fuel-pin it is an obvious choice to take \(d\) equal to the clad thickness, since the gap more or less isolates the clad on a short time scale. (In current LMFBR designs the clad thickness \(d = 0.5 \times 10^{-3} \text{ m}\); the equivalent "thickness" of the gap in terms of stainless steel is of the order of \(\lambda h_{gap} = 2 \times 10^{-3} \text{ m}\), for \(\lambda = 20\) and \(h_{gap} = 10^4\).)

The response spectrum is defined from the eigenvalue problem:

\[
    \left| -\frac{\rho c d^2}{\lambda r} [M] + [K] \right| = 0
\]

From the values of the coefficients \(m_{ij}\) and \(k_{ij}\) given in Appendix 2, the time constants \(\tau\) can be defined for different numbers of DOF taken into consideration (see Table I):

<table>
<thead>
<tr>
<th>#DOF</th>
<th>(\rho c d^2/\lambda r)</th>
<th>(\tau \times 10^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0, (1)*</td>
<td>(\infty), (50)*</td>
</tr>
<tr>
<td>1, 2</td>
<td>0, 12</td>
<td>(\infty), 4.17</td>
</tr>
<tr>
<td>1, 2, 3</td>
<td>0, 12, 60</td>
<td>(\infty), 4.17, 0.8</td>
</tr>
<tr>
<td>(\rho c = 4 \times 10^6); (d = 0.5 \times 10^{-3}); (\lambda = 20)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* see appendix 2 (MKS units)

From this table it is seen that for time steps of the order \(10^{-3}\) s and bigger, it is sufficient to take 3 DOF. The eigenvalue problem can be solved analytically and the following uncoupled equations result:

\[
    \frac{da_1}{dt} = \frac{2}{\rho c d} (q - q_c)
\]
\[
    \frac{da_2}{dt} + \frac{1}{\tau_2} a_2 = \frac{6}{\rho c d} (q - q_c)
\]
\[
    \frac{da_3}{dt} + \frac{1}{\tau_3} a_3 = \frac{30}{\rho c d} (q - q_c)
\]

\(a_1 = T_1 + \frac{1}{2} T_2 + \frac{1}{3} T_3\) \quad (average temperature of the slab)

\(a_2 = T_2 + T_3\)

\(a_3 = T_3\)

The wall temperature is given by:

\[
    T_w = a_1 + \frac{1}{2} a_2 + \frac{1}{2} a_3
\]

The parameters \(\alpha\) and \(\beta\) are defined from the analytical solution of (19) for a linear RHS during the time step \(\Delta t\):

\[
    q - q_c = q^0 - q_c^0 + (\Delta q - \Delta q_c) \frac{1}{\Delta t}
\]

The solutions are
\[ \Delta a_i = f_i + (\Delta q - \Delta a_c) g_i \quad (i = 1, 2, 3) \]  \hspace{2cm} (23)

\[ f_i = \frac{2\Delta t}{\rho c_d} (q_i^n - q_i^0) \]

\[ f_2 = \frac{6}{\rho c_d} (q_1^n - q_2^n) \tau_2 - a_2^n \left( 1 - \exp \left( -\Delta t/\tau_2 \right) \right) \]  \hspace{2cm} (24)

\[ f_3 = \frac{30}{\rho c_d} (q_1^n - q_3^n) \tau_3 - a_3^n \left( 1 - \exp \left( -\Delta t/\tau_3 \right) \right) \]

\[ g_1 = \frac{\Delta t}{\rho c_d} \]

\[ g_2 = \frac{6}{\rho c_d} \frac{\tau_2}{\Delta t} (\Delta t - \tau_2 \left( 1 - \exp \left( -\Delta t/\tau_2 \right) \right) \]  \hspace{2cm} (25)

\[ g_3 = \frac{30}{\rho c_d} \frac{\tau_3}{\Delta t} (\Delta t - \tau_3 \left( 1 - \exp \left( -\Delta t/\tau_3 \right) \right) \]

The parameters \( \alpha \) and \( \beta \) are defined by

\[ \alpha = f_1 + \frac{1}{6} f_2 + \frac{1}{6} f_3 + \beta \Delta q \]

\[ \beta = g_1 + \frac{1}{6} g_2 + \frac{1}{6} g_3 \]  \hspace{2cm} (26)

Conclusions

A method is described to couple separate modules for fuel-pin and thermohydraulics. Comparisons with the stand-alone program BLOW-3A\(^3\), which treats the hydraulics and fuel-pin simultaneously, has shown the efficiency of the present method. Problems of sodium boiling including superheat, dry-out and condensing have been treated with success.

References


APPENDIX 1

Approximate analysis of overall fuel-pin time constant

To appreciate the arguments of the paragraph "Fuel-pin modules" concerning the time steps used in the fuel-pin model, an approximate analysis is presented concerning the basic time constant of fuel-pins. To this end the eigenvalue problem related to (1) has to be solved

\[ \left| -\frac{1}{\tau} [M] + [K] \right| = 0 \]  \hspace{2cm} A1(1)

The approximate analysis consists of lumping gap, clad and film in one single resistance:

\[ \frac{1}{h^*} = \frac{1}{h_{gap}} + \frac{d}{\lambda_c} + \frac{1}{h} \]  \hspace{2cm} A1(2)

In the fuel two nodes are introduced, at the surface and at the centreline, with a parabolic temperature distribution (Fig. 2).
Fig. 2 - Simplified analysis of fuel pin with one finite element.

Following the standard procedure of the Galerkin FEM (see e.g. ref. 1) the eigenvalue problem becomes:

\[ A1(4) \]

\[ \begin{pmatrix} \frac{\rho c R^2}{12\tau} & \frac{1}{\lambda_f} \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{12\lambda_f} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \]

\[ \tau_{1,2} = \frac{\rho c R^2}{12\lambda_f} \frac{1}{1 + \frac{3}{2}N \pm \sqrt{(1 + \frac{3}{2}N)^2 - \frac{3}{4}N^2}} \]

\[ N = \frac{h^* R}{\lambda_f} \]

For current LMFBR designs:

\[ h = 10^5, h_{gap} = 10^5, d = 0.5 \times 10^{-3}, \lambda_c = 20 \]

\[ \rho c_f = 4 \times 10^6, R = 3 \times 10^{-3}, \lambda_f = 3 \]

For these values one obtains

\[ h^* = 0.7 \times 10^5, N = 7 \]

\[ \tau_1 = 2.7, \tau_2 = 0.15 \]

These time constants do indeed show that the overall response of the fuel is slow as compared to response of the clad (Appendix 2). The smaller time constant \( \tau_2 = 0.15 \) is related to the fuel surface temperature \( T_2 \) as compared to the medium temperature for variations of the heat transfer coefficient. The bigger time constant \( \tau_1 = 2.7 \) is related to the average fuel temperature for variations of the boundary conditions. The physical meaning is that thermal inertia of the pin is important. Doppler feedbacks which are related to the average fuel temperature respond slowly to changes in boundary conditions, but power to coolant more rapidly. In a similar way, the average temperature of the pin reacts fairly on a change in neutron power, but the power to coolant not.

APPENDIX 2

Response spectrum for various DOF

The matrices [M], [K] and [b] follow the Galerkin weighting procedure 1.
\[
[M] = \rho c d \begin{bmatrix}
1, \frac{1}{2}, \frac{1}{3}, & \ldots \\
\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, & \ldots \\
\frac{1}{3}, \frac{1}{4}, \ldots & m_y
\end{bmatrix}
\]

\[
m_y = \int_0^1 p_i p_j d\xi = 1/(i + j - 1)
\]

\[
[K] = \frac{\lambda}{d} \begin{bmatrix}
0 & 0 & 0 & 0 & \ldots \\
0 & 1 & 1 & 1 & \ldots \\
0 & 1 & 4 & 3 & \ldots \\
0 & 1 & & & k_{ij}
\end{bmatrix}
\]

\[
k_{ij} = \int_0^1 \frac{d}{d\xi} \frac{d}{d\xi} d\xi = \frac{(i-j)(i-1)}{i+j-3} \quad i \geq 2, j \geq 2
\]

\[
\{b\} = \begin{bmatrix}
2 \\
\frac{3}{2} \\
\frac{2}{3}
\end{bmatrix}
\]

\[
b_i = p_i(\xi = 0) + \int_0^1 p_i d\xi
\]

The response spectrum is defined by solving the eigenvalue problem. For only one DOF it does not exist \((\tau = \infty)\), since \(h\) has not been taken into account. A more physical quantity is defined from the lumped heat balance:

\[
\rho c d \frac{dT_c}{dt} + h^* T_c = h^* T_m
\]

\[
\frac{1}{h^*} = \frac{1}{h} + \frac{d}{2\lambda}
\]

\[
\tau = \frac{\rho c d}{h^*} = \frac{\rho c d^2}{\lambda} \left( \frac{1}{N} + \frac{1}{2} \right)
\]

\[
N = 2.5 \quad \text{for current LMFBR designs}
\]

\[
\frac{\rho c d^2}{\lambda \tau} \approx 1 \quad \text{(see Table I)}
\]

For two DOF the eigenvalue problem becomes:

\[
\left| -\frac{\rho c d^2}{\lambda \tau} \begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{3} \\
\frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\
\frac{1}{3} & \frac{1}{4} & \ldots
\end{bmatrix} + \begin{bmatrix}
0 & 0 & \\
0 & 1 & \ldots
\end{bmatrix} \right| = 0 \quad ; \quad \frac{\rho c d^2}{\lambda \tau} = 0.12
\]

For three DOF the eigenvalue problem becomes:

\[
\left| -\frac{\rho c d^2}{\lambda \tau} \begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\
\frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \ldots \\
\frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \ldots
\end{bmatrix} + \begin{bmatrix}
0 & 0 & 0 & \\
0 & 1 & 1 & \ldots
\end{bmatrix} \right| = 0 \quad ; \quad \frac{\rho c d^2}{\lambda \tau} = 0, 12.60
\]

In Table I the fundamental time constants for current LMFBR clad are given.

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