The CYGRO5 Fuel Rod Analysis Computer Program

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CYGRO5 is a finite element computer program for the analysis of temperatures, stresses, and deformations in an oxide fueled rod-type fuel element. It was developed from CYGRO4 by the inclusion of an explicit thermo-mechanical model for radially zoned duplex fuel; a capability for analyzing the whole rod at a single program execution; a number of improved materials models, including a temperature and fission rate dependent fission gas release model with an associated swelling model; and revised and improved numerical procedures to provide stable and reliable program operation. CYGRO5 was developed as part of the AWBA Development Program.

The model for fuel-zone-to-fuel-zone, fuel-to-clad, and rod-to-support mechanical interactions is an important feature of CYGRO5. In addition to interacting by radial stresses, the fuel zones and the fuel and cladding can interact through axial forces. The fuel and cladding axial strain rates can be the same or different, depending on gap sizes, the direction and magnitude of the axial interaction forces, and the effects of pellet "hourgassing," eccentric pellets, lodged chips, and cladding collapse, where the effects are relevant. These interactions are particularly important in the correct representation of rod behavior in response to reactor power changes such as those encountered in "peak load following" operation. The program is adapted to analysis of rods with duplex fuel, single zone fuel, or both. Single zone fuel can be solid or annular. In dual zone fuel the two zones can have different axial strains, depending on the results of the analysis. The model for interaction between the fuel zones is similar to that for interaction between the outer fuel zone and the cladding. When the program is applied in the analysis of a whole rod it considers the effects of axial variations in fission rate, fast neutron flux, and axial communication of fill and fission gasses but neglects effects arising from axial conduction of heat or mechanical interactions between segments.

The revised materials models include representations for cladding elastic anisotropy, thermally activated recovery of irradiation growth, a more general form of stress dependence in cladding creep than in previous CYGRO programs, and a temperature and fission rate dependent transient gas release and retained gas dependent fuel swelling model. The gas release and fuel swelling model is a simplified adaptation of the one developed by C. C. Dollins.

A revised procedure for solving the coupled fuel temperature and fuel-to-clad gap size equations has provided significantly improved program reliability. This illustrates the point that the neglect of interaction effects can lead to unexpected numerical instabilities.
1. Introduction

The CYGRO5 computer program performs a coupled analysis of temperatures, stresses, and deformations in an oxide fueled rod-type fuel element using the Finite Element Method. CYGRO5 was developed from CYGRO4 /1/ by expanding the program's capabilities, refining its models, and improving its numerical procedures.

Chief among the new capabilities are an explicit thermo-mechanical model for radially zoned duplex fuel and the capability to analyze the whole rod at a single program execution, accounting for the effects of axial variations in power, temperature, and fission gas release and the axial transport of fission gas. The program retains the capability for analyzing single zone fuel, and a rod can have both single zone and duplex fuels.

The refined materials models include representations for cladding elastic anisotropy, thermally activated recovery of irradiation growth, a more general form of stress dependence in cladding creep, and a temperature and fission rate dependent, transient fission gas release model with an associated retained gas dependent fuel swelling model. The gas release and fuel swelling model is a phenomenological adaptation from the model developed by Dollins /2/.

The most important revision to the numerical procedures is a new method for solving the coupled fuel temperature, fuel-clad gap size, and fuel-fuel gap size equations. The revised solution procedure eliminated a computational instability that had plagued both CYGRO3 and CYGRO4.

CYGRO5 is fully documented in Reference /3/. This paper can only call attention to developments embodied in the program. We shall focus on the analysis of radially zoned duplex fuel and the improved solution of the coupled fuel-clad gap and fuel temperature equations.

2. Radially Zoned Duplex Fuel

In CYGRO5's representation of duplex fuel the two fuel regions are treated as separate, homogeneous regions with distinct material properties. Each finite element in the fuel has its own fission rate, heating rate and fission depletion, as determined by independent nuclear analysis. All fuel material responses are taken as functions of the local stress, fission rate, temperature, et cetera as appropriate.

The two fuel zones and the clad are viewed as independent substructures. By applying the equations of continuity and equal action and reaction between the finite elements comprising these substructures it is possible to express the external dimensions of the substructures in terms of the forces that act on them. In each substructure all finite elements have the same length and, thus, axial strain. The lengths and axial strains of the two fuel zones may be the same or different depending on problem input and the results of computations. Each zone is represented as a tube whose ends and inner and outer surfaces are subjected to the pressure existing in the interior of the rod.1 Additional stresses arise from the mechanical interaction between the fuel zones and the fuel and clad. Let the radial interaction force between the fuel zones be denoted by $F_1$ while the axial interaction force between the fuel zones is $F_2$. Similarly, the radial interaction force between the outer fuel zone and the clad is $F_3$ and the axial interaction force between the outer fuel zone and the clad is $F_4$. Finally, the axial interaction force between the rod and the support is $F_5$.

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1 A solid fuel zone is represented as a tube with zero inner radius. This automatically achieves the appropriate structural response.
The numbering for the lengths is as follows: the length of a section of fuel in the central zone is $l_1$, the length of a corresponding section of fuel in the outer zone is $l_2$, the length of a corresponding section of the clad is $l_3$, and the length of a corresponding section of support is $l_4$. Finally, the inner radius of the central fuel zone is $a_1$, while its outer radius is $b_1$, the inner and outer radii of the outer fuel zone are $a_2$ and $b_2$, respectively, and the inner radius of the clad is $a_3$. Interaction between the two fuel zones, between the outer fuel zone and the clad, and between the rod and the support is characterized by the interaction forces $F_i$, $i=1, \ldots, 5$, and the relative dimensions $V_i = a_i - b_i$, $V_2 = l_2 - l_1$, $V_3 = a_3 - b_2$, $V_4 = l_3 - l_2$, and $V_5 = l_4 - l_3$, which correspond to the gap between the two fuel zones, the difference between the lengths of the two fuel zones, the gap between the clad and the outer fuel zone, the difference between the lengths of the clad and the outer fuel zone, and the difference between the lengths of the support and the rod.

The substructure relations for the fuel zones and the cladding provide five equations relating the five interaction forces $F_i$, $i=1, \ldots, 5$ to the five relative dimensions $V_i$, $i=1, \ldots, 5$. Five other equations are needed to obtain a solution for the $F_i$ and $V_i$. These equations are obtained from the current status of interaction between fuel zones, between the outer fuel zone and the cladding, and between the rod and the support.

Radial interactions occur when $V_1$ or $V_3$ is zero. When there is radial interaction, the corresponding interaction force, $F_1$ or $F_3$, must be positive. The presence of a gap corresponds to positive $V_1$ or $V_3$. In that case the corresponding interaction force, $F_1$ or $F_3$, must be zero. These criteria provide the basis for a pair of additional equations governing $F_1$ or $V_1$ and $F_3$ or $V_3$.

There are three possible states of axial interaction between the fuel zones, between the outer fuel zone and the clad, and between the rod and support ($i=2, 4$, or $5$): $dV_i/dt = 0$, $dV_i/dt > 0$, and $dV_i/dt < 0$. In the first case the magnitude of $F_i$ is limited. In the second and third cases the magnitude of $F_i$ is known, and the sign is specified so that the product $F_i dV_i/dt < 0$. This reflects the fact that friction results in the dissipation of mechanical energy. These considerations provide three further equations governing $F_1$ or $V_1$ for $i=2, 4$, and $5$.

The solution of the five interaction equations involves an iteration procedure in which the interaction state is assumed, the resulting structural response is calculated, the results are compared with the requirements of the assumed interaction state, and the interaction assumption is changed as required. This process continues until a fully consistent interaction assumption is found and the resulting structural response is calculated. The details of this interesting and important process are discussed fully in References /1/ and /3/.

The slippage loads, $F_2$ and $F_4$, depend on a number of parameters. These include the effects of direct radial interaction through a coefficient of friction acting with $F_1$ or $F_3$ as appropriate, the effects of partial radial interaction due to pellet "hourglassing", and the effects of pellet eccentricity or lodged chips. The predicted length changes in fuel and cladding are sensitive functions of these parameters.

The duplex fuel analysis capability in CYGROS has received extensive use in the AWBA Development Program. It has been important to the correct analysis of observed deformations.
3. Elimination of Numerical Instability in Calculating Gap Temperature Drop

Although the original version of CYGRO4 /1/ was much more reliable than CYGRO3 /4/, it would occasionally fail to complete analyses of high power rods. Examination of detailed output indicated that these failures were associated with uncontrolled oscillations in the numerical results. These uncontrolled oscillations appeared as the fuel-clad gap was closing either on an up-power transient or as the fuel swelled and the cladding decreased in diameter due to creep. The cause of the uncontrolled oscillations was unknown. Although they might have reflected a deficiency in the mathematical models in CYGRO4, their general character suggested that they resulted from an instability in the solution procedure. This conclusion was based on the fact that uncontrolled oscillations occurred even though the time steps were made arbitrarily small and on the fact that the initial stages of the oscillation displayed an increasing amplitude that appeared to represent a geometrical progression in which each oscillation was larger than the previous one by a fixed proportion.

Since the CYGRO mathematical model is so complex and its solution procedure is so involved, a simple model with a number of the features of the CYGRO model was used to investigate the stability of the CYGRO solution procedure. This simplified the work involved and led to an independent analysis that predicted the onset of uncontrolled oscillations. This success suggested that the uncontrolled oscillations could be prevented by comparatively simple modifications to the CYGRO4 computer program. The modified program never displayed the uncontrolled oscillations, and the revised solution procedure was applied in CYGRO5 with equal success. This section provides a precis of the stability analysis and the revised solution procedure. The interested reader may wish to refer to Reference /3/ for a fuller discussion.

To illustrate the mathematics, consider a greatly simplified model problem, the analysis of a fuel element with a linearly elastic fuel region whose thermal expansion coefficient, \( \alpha_f \), and thermal conductivity, \( C_f \), are independent of temperature. When the heat generation rate per unit length is \( q \) and the surface temperature of the fuel is \( T_f \), the radius is

\[
r_f = R_f \left( 1 + \alpha_f (T_f + \frac{q}{8\pi C_f}) \right),
\]

where \( R_f \) is the radius for \( T_f = 0 \) and \( q = 0 \). Assuming that the thermal conductivity of the fill gas dominates heat transfer across the fuel-clad gap,

\[
T_f = T_c + \frac{q}{\pi (T_f + r_f) r_f C_f} \frac{g + r_f c_{l} r_f}{K(T_c - T_f)^m},
\]

where \( T_c \) is the temperature at the inner surface of the cladding, \( r_c \) is the radius of the inner surface of the cladding, \( g \) is a "jump distance" associated with wall roughness and gas-solid energy transfer, and the thermal conductivity of the gas at temperature \( T \) is \( (2mK(T)^m) \). For the present purpose we shall assume that \( T_c \) and \( r_c \) are independent of \( q \) and that \( r_f < r_c \). Under these conditions the problem of calculating the surface temperature of the fuel reduces to solving Eqs. (1) and (2) for \( T_f \) and \( r_f \) at the given value of \( q \) for known \( \alpha_f, C_f, R_f, g, T_c, T_f, K, \) and \( m \).

This is equivalent to finding the roots \( T = T_f \) and \( r = r_f \) of the simultaneous equations

\[
F(r, T; q) = 0
\]

2 This difficulty was also observed with CYGRO3.
and
\[ G(r, T; q) = 0 \]  
(4)

where
\[ F(r, t; q) = r - R_f a_f T - \frac{R_f a_f q}{B C_f} \]  
(5)

and
\[ G(r, T; q) = T - T_c + \frac{q(g + r - r)}{K(T_c + T)^2}. \]  
(6)

In the CYGRO programs the analysis starts from a known state \( q = 0 \) at \( t = 0 \) and obtains an approximate solution at each of a succession of later times, \( t = t_k, k = 1, \ldots, N \) with \( t_k < t_{k+1} \), using specified values \( q_k = q(t_k) \). In the original gap-size-dependent gap-temperature-drop model of Reference /4/ the solution process started with an iterative solution of Eq. (4) for \( T = T_f \), holding \( r = r_k \) fixed. That solution provided the basis for estimating \( dT_f/dt \) for given \( dq/dt \), neglecting any effect of the change in gap size. The resulting value of \( dT_f/dt \) was used to compute \( dr_f/dt \), including a correction term to reduce the errors associated with Simpson's rule integration of the thermal strain rate.\(^3\) The correction term introduced in CYGRO3 corrected the calculated thermal strain based on a calculation of the correct thermal strain for the current temperature but did not apply the correction until the next time step. To describe the solution procedure precisely, consider its application to the model problem. The fuel surface temperature was calculated by solving
\[ G(r_k, T; q_k) = 0 \]  
(7)

for \( T_k \). Then, approximating the derivative of \( q \) for \( t_k < t < t_{k+1} \) as
\[ q = (q_{k+1} - q_k)/(t_{k+1} - t_k), \]  
the derivative of \( T \) was approximated by
\[ \frac{\dot{T}}{T} = \left( \frac{\partial G}{\partial T} \right)_{t=t_k}^{-1} \frac{\partial G}{\partial q} q_k. \]  
(8)

For \( t = t_k \) and \( T = T_k \), the correct radius is \( r_k \), which can be found by solving
\[ F(r_k, T_k; q_k) = 0. \]  
This was used with
\[ \frac{\dot{r}}{r} = -\frac{\partial F}{\partial q} q_k - \frac{\partial F}{\partial T} \dot{T} \]  
(9)

to compute
\[ r_{k+1} = r_k + (F - g) + q_k \left[ \frac{\partial F}{\partial q} + \frac{\partial F}{\partial T} \dot{T} \right] (t_{k+1} - t_k). \]  
(10)

The variable \( \rho \) is calculated from the thermal expansion rate by Simpson's rule:
\[ \rho_{k+1} = \rho_k + q_k \left[ \frac{\partial F}{\partial q} + \frac{\partial F}{\partial T} \dot{T} \right] (t_{k+1} - t_k). \]  
(11)

The extreme simplicity of the model problem considered here may make the set comprising Eqs. (8), (10) and (11) seem awkward. It should be remembered that the complex structure of CYGRO made it difficult to discern the structure of the solution procedure,

\(^3\) The error from using Simpson's rule is of the same sign in every time step. It can reach substantial values, especially in analyses of cyclic operation at alternating high and low power levels.
which had evolved through a sequence of developments that were natural, or at least tempting, ones as the capabilities of the program were extended and operational problems were resolved. The solution procedure worked well for most cases even though it was subject to the instability that is the topic of this section.

To facilitate the stability analysis, note that by subtracting Eq. (11) from Eq. (10) we obtain

$$ r_{k+1} - \rho_{k+1} = r_k - \rho_k. $$

This will be used in place of Eq. (10). Now, writing the exact solution at $t = t_m$ as $r_m^*, T_m^*$ we use Taylor's series to write

$$ \frac{\partial G}{\partial t}\bigg|_{\text{exact}} (r_{k+1} - r_{k+1}^*) + \frac{\partial G}{\partial T}\bigg|_{\text{exact}} (T_{k+1} - T_{k+1}^*) + \ldots = 0 $$

instead of Eq. (6), indicating higher order terms by the dots. Likewise, Eq. (12) becomes

$$ (r_{k+1} - r_{k+1}^*) - (\rho_{k+1} - \rho_{k+1}^*) = (r_k - r_k^*) - (\rho_k - \rho_k^*). $$

Moreover, since $F(\rho_m^*, T_m^*) = 0$, and both $\rho_{k+1}$ and $\rho_{k+1}^*$ are defined by Eq. (11), so that the terms in $q_k$ appear equally in both,

$$ \rho_{k+1} - \rho_{k+1}^* = \rho_k - \rho_k^* + \ldots $$

The solution is stable provided an error at $t = t_k$ is not magnified in the step from $t_k$ to $t_{k+1}$. Thus, to investigate the stability of the original gap temperature drop solution procedure consider its response to the errors $\epsilon T_{k+1} = T_k - T_k^*$ and $\epsilon r_{k+1} = r_k - r_k^*$. The asymptotic response at $\epsilon T_{k+1} = \epsilon r_{k+1} = \epsilon r_{k+1}^* = 0$ can be determined by neglecting the higher order terms in Eqs. (13), (14), and (15) and solving for $\epsilon T_{k+1}$, $\epsilon r_{k+1}$ and $\epsilon r_{k+1}^*$. The result is

$$
\begin{bmatrix}
\epsilon T_{k+1} \\
\epsilon r_{k+1} \\
\epsilon r_{k+1}^*
\end{bmatrix} =
\begin{bmatrix}
\frac{\partial G}{\partial T} \left( \frac{\partial G}{\partial T} \right)^{-1} \frac{\partial F}{\partial \rho} - \frac{\partial G}{\partial T} \left( \frac{\partial G}{\partial T} \right)^{-1} \frac{\partial G}{\partial T} \left( \frac{\partial G}{\partial T} \right)^{-1} \\
- \frac{\partial F}{\partial \rho} \frac{\partial G}{\partial T} \left( \frac{\partial G}{\partial T} \right)^{-1} 1 & -1 & 0 \\
- \frac{\partial F}{\partial \rho} \frac{\partial G}{\partial T} \left( \frac{\partial G}{\partial T} \right)^{-1} 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\epsilon T_k \\
\epsilon r_k \\
\epsilon r_k^*
\end{bmatrix}
$$

This result has been simplified by using $\partial F/\partial \rho = 1$ and the fact that $\epsilon r_{k+1} = \epsilon r_{k+1}^* = (\partial F/\partial \rho)^{-1} (\partial F/\partial T) \epsilon T_k$. The magnitude of the error at $t = t_{k+1}$ is greater than that at $t = t_k$ whenever the matrix in Eq. (16) has an eigenvalue of larger than unit magnitude. This can happen when the eigenvalue $S = (\partial G/\partial \rho) (\partial G/\partial T)^{-1} (\partial F/\partial T)$ attains a large magnitude as it can for relatively large values of $q_k$ or for small values of $r_C r_f$, the gap size. Since $S$ can be shown to be inherently negative, the instability will be one involving an oscillation of steadily growing amplitude, which was the case in the CVGRO problems in which program failure occurred.

These results prompted experimental modifications to compute the value of $S$ from the finite element data in the program. This made it possible to test the stability

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4 See Reference /5/, especially Chapter I, Section 1.
for perfectly general problems instead of just for the simple model problem discussed here. The results were gratifying; all problems known to oscillate did so only when the magnitude of $S$ exceeded 1.0. Moreover, other problems that had not been known to display oscillations were found to have them. The difference between fatal and non-fatal oscillations appeared to lie in the rate at which the gap was closing, but this was not investigated, since the objective was to eliminate the instability completely.

The instability was eliminated by revising the solution procedure to calculate $T_\delta$ while accounting for the effects of $T_\delta$ on the size of the fuel and, thus, the gap. In concept this corresponds to simultaneous solution of $F(r_\delta T_\delta; q_\delta) = 0$ and $G(r_\delta T_\delta; q_\delta) = 0$ rather than solving $G(r_\delta T_\delta; q_\delta) = 0$ for $T_\delta$ at fixed $r$ followed by calculating the value of $r_\delta$ from $T_\delta$ through solution of $F(r_\delta T_\delta; q_\delta) = 0$. The merit of this is apparent. In fact, it increased the internal consistency of the program by solving all the equations with the procedures used to solve the structural equations. The details of the program modifications are too involved for presentation here. The interested reader will find them in Section IV of Reference /3/. The central point to be made here is that the revised solution procedure has been fully reliable in solving all gap-size-dependent gap-temperature-drop analysis, which are the standard cases for both CYGR04 and CYGR05.

The results presented here tell a cautionary tale to program developers. Numerical instabilities can easily arise when new program capabilities are added and changes are made to correct modeling or calculational deficiencies. At those times, when everyone wants a "quick fix" to a deficiency or an operational problem, it is natural to overlook the need to fit the changes in so that the program's solution procedure functions as planned. The resulting instabilities may bear no relation to the physics of the model and may appear only infrequently. Unfortunately, when they do occur they are likely to prove difficult to find unless one is very lucky.

We are indebted to Dr. L. A. Hageman and Dr. M. M. Sussman of Bettis Atomic Power Laboratory for the essential guidance they gave to the effort that produced the analysis presented here.

4. Conclusion

The development of CYGR05 has provided a substantial increment of program capabilities, modeling, and program reliability beyond CYGR04. These were of substantial importance in the ANS/ Development Program at the Bettis Atomic Power Laboratory, operated by Westinghouse Electric Corporation for the United States Department of Energy.
References


