FUEL THERMAL/MECHANICAL BEHAVIOUR UNDER LOSS OF COOLANT ACCIDENT CONDITIONS AS PREDICTED BY THE *FACTAR* CODE

C.J. WESTBYE, A.C. BRITO, J.C. MACKINNON, H.E. SILLS and V.J. LANGMAN

Ontario Hydro
Reactor Safety and Operational Analysis Department
700 University Avenue, Toronto, Ontario M5G 1X6

ABSTRACT

FACTAR (Fuel And Channel Temperature And Response) is a computer code developed to simulate the transient thermal and mechanical behaviour of 37-element or 28-element fuel bundles within a single CANDU fuel channel for moderate (i.e., sheath temperatures less than the mleting point of Zircaloy) loss-of-coolant accident (LOCA) conditions including transition and large break LOCAs with emergency coolant injection assumed available. FACTAR's predictions of fuel temperature and sheath failure times are used for subsequent assessment of fission product releases and fuel string expansion. In this paper, model capabilities and calculated quantities of the code are summarised. The results from overly severe test cases are presented in order to clearly demonstrate the effect on calculated fuel channel behaviour of a mechanistic assessment of fuel-to-sheath heat transfer, and the impact of using a diffusion-limited model for Zircaloy/steam reaction (i.e., FROM) as opposed to a reaction rate correlation, coupled with the assumption of unlimited steam supply.

1. INTRODUCTION

FACTAR (References 1-4) is a computer code developed to simulate the transient thermal and mechanical behaviour of 37-element or 28-element fuel bundles within a single CANDU fuel channel for moderate loss-of-coolant accident (LOCA) conditions including transition and large break LOCAs with emergency coolant injection (ECI) assumed available. The code has been designed to characterize the transient phenomena of sheath strain and dynamic blowdown cooling conditions throughout a LOCA, including any initial overpower transient. FACTAR provides a detailed transient model of sheath deformation and the impact of sheath strain on fuel-to-sheath heat transfer and consequently the radial temperature profiles within the fuel elements. FACTAR's predictions of fuel temperatures and sheath failure times are used for subsequent assessment of fission product release. FACTAR has been designed to supersede CHAN (Reference 5) for analysis of a range of moderate accidents, defined as those which avoid severe fuel damage conditions (which include gross bundle deformation (*e.g.*, bundle slumping), significant molten material formation and significant hydrogen production). FACTAR has been used at Ontario Hydro for transition and large break LOCA analyses, including fuel string compression studies, and at New Brunswick Power for investigation of fuel string compression in a large break LOCA.

The basis for FACTAR is the validated code ELOCA.Mk4 (References 6,7), which is used to perform detailed fuel element calculations for a representative fuel element of each fuel pitch circle in each bundle in a single channel. Channel thermal hydraulic conditions are calculated using a flow-ring model driven by input inlet transients, typically calculated from a sophisticated system thermal hydraulic code (*e.g.*, TUF (Reference 8)). Convective heat transfer coefficients, thermal radiation fluxes (calculated using a ring/ring model) and

steam flow rates (used to calculate Zircaloy/steam reaction rates) are calculated by the thermal hydraulic and fuel channel portion of FACTAR and passed as boundary conditions to the fuel model ELOCA. Steady-state burnup-dependent fuel element characteristics are calculated by the code FACTAR_SS (Steady-State) (Reference 9), which was developed from ELESIM-II (MOD10) (Reference 10) to provide initial conditions for transient calculations performed with FACTAR.

In addition to summarizing model capabilities and calculated quantities, this paper presents test cases which demonstrate the effect of incorporating a mechanistic assessment of the fuel-to-sheath heat transfer coefficient, and the impact of using a diffusion-limited model for Zircaloy/steam reaction (*i.e.*, FROM (Reference 11)) as opposed to a reaction rate correlation. Inclusion of these detailed models is shown to have a significant impact on predicted fuel temperatures, and should not be ignored in the analysis of fuel channel behaviour.

2. SUMMARY OF MODELS

2.1 Overview

The discussion of models presented here focuses on the most recently released code version FACTAR 1.3.1, which evolved under the revision control process from FACTAR 1.2. FACTAR 1.3.1 was developed to incorporate enhanced quality assurance features (*e.g.*, automatic version identification), enhanced performance by code optimisation, and modelling improvements primarily impacting upon pressure tube thermal behaviour. Modelling assumptions include: homogeneous two-phase flow, circumferential symmetry, a ring/ring geometry applied for thermal radiation calculations, no severe geometry changes during the transient (*i.e.*, only pressure tube and sheath strain are considered), uni-directional flow, with the flow direction remaining the same throughout the transient (except during the initial blowdown period, during which fuel element calculations are driven by TUF calculations).

Initial conditions and channel boundary condition transients provided externally include:

- coolant pressure, inlet coolant enthalpy and mass flow rate (from a system thermal hydraulics code);
- fuel power transients (from a physics code);
- initial fuel and sheath conditions (power and burnup history dependent) including element internal pressure, temperature distribution and oxide layer thickness (from FACTAR_SS).

FACTAR output for both fuel and thermal hydraulic characteristics is available. Information required to calculate fission product release, including UO_2 temperature transients and sheath failure times, is output for subsequent analysis. Additional information which primarily relates to general channel behaviour (such as pressure tube temperature and strain, coolant characteristics, hydrogen produced) is also output. See References 1 to 3 for more details.

2.2 Thermal Hydraulic and Channel Model

The calculation proceeds node by node (from inlet to outlet) along the length of the channel at each time step, with the inlet enthalpy for the current bundle dependent upon the outlet enthalpy from the adjacent upstream bundle. The coolant is modelled as flowing in annuli bounded by each fuel pitch circle and by the pressure tube. The flow distribution between annuli at the inlet to the bundle is calculated from Bernoulli's equation. The fraction of fuel element surface area in contact with each bounding flow annulus changes with time due to sheath strain. The mixing characteristics between flow annuli and at bundle endplates must be specified; a total of five options are available. An ongoing assessment of flow visualization studies and comparison with the predictions of ASSERT-PV (Reference 12) to assist in establishing coolant mixing characteristics is in progress.

The change in coolant enthalpy as a function of axial location, radial location and time is evaluated by

solution of the one-dimensional, transient coolant energy conservation equation. The heat transfer rate to a given flow annulus in contact with surfaces of fuel elements from a fuel ring is evaluated using the sheath surface temperature evaluated in ELOCA and the appropriate coolant temperature and sheath-to-coolant convective heat transfer coefficient. The amount of steam in a given annulus, calculated from the coolant thermodynamic quality, is used to provide a boundary condition for the exothermic Zircaloy/steam reaction calculation. The steam flow rate is modified, according to the mixing model, to account for oxygen depletion through reaction at upstream bundle locations.

The calculation of the convective sheath-to-coolant heat transfer coefficient depends on the dryout status at the current axial location. The location of the dryout front is determined when the average convective heat flux from all elements in the bundle exceeds the bundle-average critical heat flux; dryout is assumed to occur at the current axial location and at all downstream bundles. Dryout at the pressure tube surface is calculated separately in FACTAR 1.3.1. For pre-dryout surfaces, a modified Dittus-Boelter equation is used which accounts for flow rate variations. For post-dryout heat transfer, the Groeneveld-Delorme correlation (Reference 13), which accounts for thermal non-equilibrium effects, is used for fuel element surfaces while the Hadaller correlation (Reference 14) is used for the pressure tube and for fuel element surfaces in contact with superheated steam. Separate calculations are performed on the inward- and outward-facing side of each fuel element, since different conditions in each of the bounding flow annuli can result in different convective heat transfer coefficients and coolant sink temperatures.

The radial pressure tube and calandria tube temperature distributions at any axial location are found by solution of the discretised one-dimensional, transient energy equation. Pressure tube strain calculations, based on the pressure tube temperature, are performed unless limited by pressure tube/calandria tube contact around the circumference. The pressure tube diameter affects the flow distribution within the bundle due to changes in the cross-sectional flow area for the outer flow annulus. The mechanical model, an implementation of Shewfelt's equations for the transverse strain of Zr-2.5wt%Nb pressure tubes (Reference 15), is coupled with the temperature solution. Radiation heat transfer calculations are performed when the coolant quality between two exchanging surfaces is greater than 90 percent. The net radiative heat flux, calculated assuming a ring/ring geometry (*i.e.*, concentric infinitely long cylinders), is applied as a surface boundary condition for each fuel element and pressure tube.

2.4 ELOCA Fuel/Sheath Model

The detailed mechanistic fuel code ELOCA.Mk4 is used as a basis for FACTAR. Calculated quantities for ELOCA.Mk4, which applies an axi-symmetric geometry to a single fuel element, include: thermal, plastic and elastic sheath deformation, variation of internal gas pressure, change in fuel characteristics (expansion, cracking and melting), radial temperature profiles, and chemical reaction between the Zircaloy sheath and steam. Modifications to the ELOCA code required to integrate it into FACTAR are summarised in References 1 to 4. Details of the extensive validation performed for ELOCA.Mk4 (and ELESIM) are summarised in Reference 2.

In FACTAR, the Zircaloy/steam reaction can either be calculated using a kinetic correlation (*i.e.*, Urbanic-Heidrick correlation (Reference 16), Sawatzky correlation (Reference 17), or Prater-Cathcart correlation (References 18, 19)), or the Full Range Oxidation Model (FROM). The validated model FROM provides a detailed representation of the Zircaloy/steam reaction at the sheath surface, considering the possible limiting effect of oxygen diffusion through the reacted sheath to unoxidised Zircaloy. The calculations are based on the solution of the moving boundary diffusion problem, explicitly accounting for the formation and deletion of beta-zircaloy, oxygen-stabilised alpha-zircaloy and ZrO_2 substrate layers.

FACTAR incorporates a mechanistic assessment of the fuel-to-sheath heat transfer coefficient. This heat transfer coefficient includes: i) a conductance term for solid-to-solid contact, taking into account the relative surface roughnesses, ii) a gas conduction term, accounting for conductivity variations in the filling gas/fission

gas mixture and a calculation of the temperature jump distance (which compensates for gas molecule/surface collisions), and iii) a term for radiant heat transfer between surfaces.

3. DEMONSTRATION ANALYSIS

FACTAR models a number of effects which are fundamentally important to the accurate representation of fuel thermal/mechanical behaviour under loss-of-coolant accident conditions. Features which have a significant impact are the variation in fuel-to-sheath heat transfer as a result of fuel and sheath mechanical deformation, and the representation of the exothermic Zircaloy/steam reaction at the sheath surface by a mechanistic, diffusion-limited model. In FACTAR, a variable fuel-to-sheath heat transfer coefficient (h_{fs}) is automatically calculated, while the use of FROM is the recommended Zircaloy/steam reaction treatment. Representation of these phenomena in other simulation codes has often assumed a constant value of h_{fs}, and used a reaction rate correlation for calculating the heat of reaction due to sheath oxidation. This section demonstrates the large impact that these assumptions have on simulation results. The case assessed was deliberately made more severe than expected for a large break LOCA with ECI available in order to clearly demonstrate the effects of variable h_{fs} and oxygen diffusion on predicted fuel and sheath temperatures. The simulations were performed using FACTAR 1.3.1 with different model options (selected via input). Three cases were studied: i) invoking the mechanistic model FROM to calculate the Zircaloy/steam reaction and internally calculating a time-variant fuel-to-sheath heat transfer coefficient (referred to as "Nominal Case"); ii) using the Prater-Cathcart correlation to assess Zircaloy/steam reaction rate, with a varying h_{fs} (referred to as "Correlation Case"); and iii) setting the fuel-to-sheath heat transfer coefficient for all fuel elements in the channel to a constant value of 10 kW/m^2.K and using FROM (referred to as "Constant hfs Case").

3.1 Case Conditions

The channel pressure, inlet enthalpy and power transients of the case presented in this demonstration analysis are typical of a 7.0 MW channel in the inner zone of Bruce Nuclear Generating Station B with a 35 percent pump discharge break occurring at the beginning of the transient. The coolant flow transient is also typical of these conditions, except in the period from 20 seconds to approximately 45 seconds, where the flow rate was reduced to lower values, *i.e.*, it is stylized. This modification to the large break LOCA conditions was made in order to achieve higher fuel and sheath temperatures, which magnifies differences arising from the modelling treatment. As a result, the temperatures reported in this paper are not representative of cases used in large break LOCA safety analyses. The input boundary conditions (channel pressure, inlet enthalpy, coolant flow rate and overpower transient) are shown in Figures 1(a) through 1(d), respectively.

The partial mixing mode was used, *i.e.*, the coolant flow is divided radially into two annuli separated by the outermost ring of fuel elements. It is assumed that there is no communication between these coolant annuli. A thermal hydraulic calculational time step of 0.1 seconds was used to a final simulation time of 150 seconds.

3.2 Effect of Zircaloy Oxidation Model

To evaluate the effect of the Zircaloy oxidation treatment, the results from the "Nominal Case" and the "Correlation Case" are compared. Figure 2 shows the sheath temperature transients predicted by FACTAR 1.3.1 for each representative fuel element at bundle 8. The results are indistinguishable until approximately 40 seconds, when the sheath temperature predicted using the Prater-Cathcart model increases by over 1000 °C compared to that predicted using FROM. A similar departure is noted for the fuel average temperature shown in Figure 3 for the same elements at bundle 8. At 40 seconds, the sheath temperature reaches a level (about 1500°C) after which the oxidation reaction becomes self-sustaining, leading to run-away oxidation and a very large sheath temperature excursion (the Prater-Cathcart model is comprised of two correlations which switch at 1510°C). The fast rate of the oxidation reaction is most clearly seen in Figure

4, which shows the total reacted layer thickness (ZrO_2 plus oxygen-stabilised alpha-Zircaloy) as a function of time. At approximately 40 seconds, the reacted layer thickness predicted by Prater-Cathcart increases dramatically, with the sheath quickly consumed. In contrast, the FROM predictions show a slow increase in reacted layer thickness, a result explained by the modelled limiting effect of oxygen diffusion through the sheath on the oxidation rate. Without such a limitation on oxygen availability at the surface of unoxidised Zircaloy, correlations (such as Prater-Cathcart) can significantly overpredict fuel and sheath temperatures.

3.3 Effect of Varying Fuel-to-Sheath Heat Transfer Coefficient

The effect of a varying h_{fs} on fuel element behaviour versus a constant value was evaluated by comparing the results from the "Nominal Case" to the "Constant hfs Case". Figure 5 shows that FACTAR predicts a much greater value of h_{fs} than the constant value of 10 kW/m^2.K for the inner two rings of fuel elements; the opposite is found for the outer two rings (for the majority of the transient for the intermediate ring). The explanation for the behaviour in the outer two rings is sheath lift-off: the internal gas pressure and differential thermal expansion between the fuel and the sheath are sufficient to cause sheath ballooning and a relatively large radial gap (about 22 μm and 187 μm for the intermediate and outer ring, respectively) between the fuel and the sheath, consequently reducing the predicted heat transfer coefficient to a low value. The effect of high h_{fs} values leading to enhanced heat removal from the fuel is apparent from Figure 3 - the fuel average temperature for the inner two rings is lower for the "Nominal Case". Figure 2 shows that higher sheath temperatures are also predicted when the h_{fs} is reduced; the sheath has stronger thermal coupling with the fuel than with the coolant, and the temperature rises as a result of the higher fuel surface temperature.

Figure 3 shows that the fuel temperature for the intermediate ring is higher for the "Constant hfs Case" than the "Nominal Case". Early in the transient, during the peak overpower period, the "Nominal" h_{fs} is larger than the constant value as shown in Figure 5; this time period is sufficiently long to lower the fuel temperature (and raise the sheath temperature) and these differences persist throughout the transient. The sheath temperature difference is enough to cause rapid oxidation of the sheath in the "Constant hfs case" which also contributes to the higher fuel and sheath temperatures.

It should also be noted that the outer ring sheath temperatures for the "Constant hfs Case" are higher than calculated in the "Nominal Case". This result is explained by considering thermal radiation exchange with the hot intermediate ring sheaths, and convective heat removal differences due to upstream effects. Since the sheath temperature tends to be higher in the "Constant hfs Case", more energy is deposited in the coolant at upstream axial locations. When the coolant reaches bundle 8, it is approximately 100°C to 200°C hotter than in the "Nominal Case". This high coolant temperature is a less effective sink for convection, and contributes to higher sheath temperatures at bundle 8.

4. CONCLUSIONS

A summary of FACTAR's model components and a demonstration analysis has been presented. The effect of the treatment of Zircaloy/steam reaction and variable fuel-to-sheath heat transfer on fuel element characteristics has been demonstrated. The use of a reaction-rate correlation for Zircaloy/steam reaction, as opposed to an oxygen-limited diffusion model, can lead to large over-predictions of fuel and sheath temperatures. The same effect is observed for the use of a constant fuel-to-sheath heat transfer coefficient, as opposed to a mechanistic model which takes into account differential thermal strain and pressure driving forces. Use of these simplified treatments (*i.e.*, constant h_{fs} and instantaneous oxygen diffusion) will, in general, lead to large overestimates of fuel and sheath temperatures and hence fission product release source terms.

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FIGURE 1
Boundary Conditions Applied for all Cases

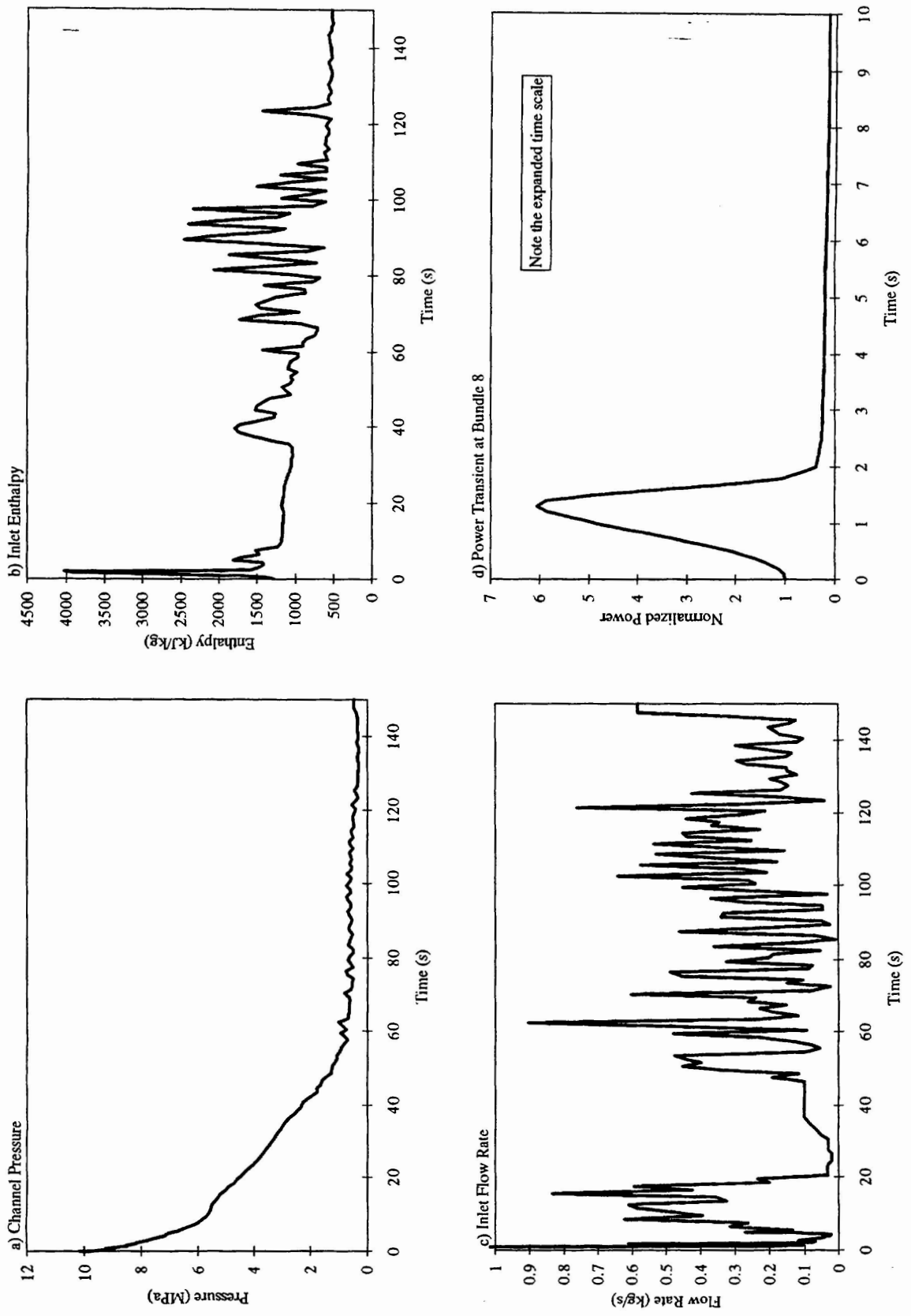

FIGURE_1.XLS/11/2/95/4:25 PM

FIGURE 2
Sheath Temperature at Bundle 8

Note: The severity of this transient is not typical of what is expected for large break LOCAs with ECI available.
The conditions analyzed were deliberately more severe in order to clearly indicate the effects of hfs and oxygen diffusion.

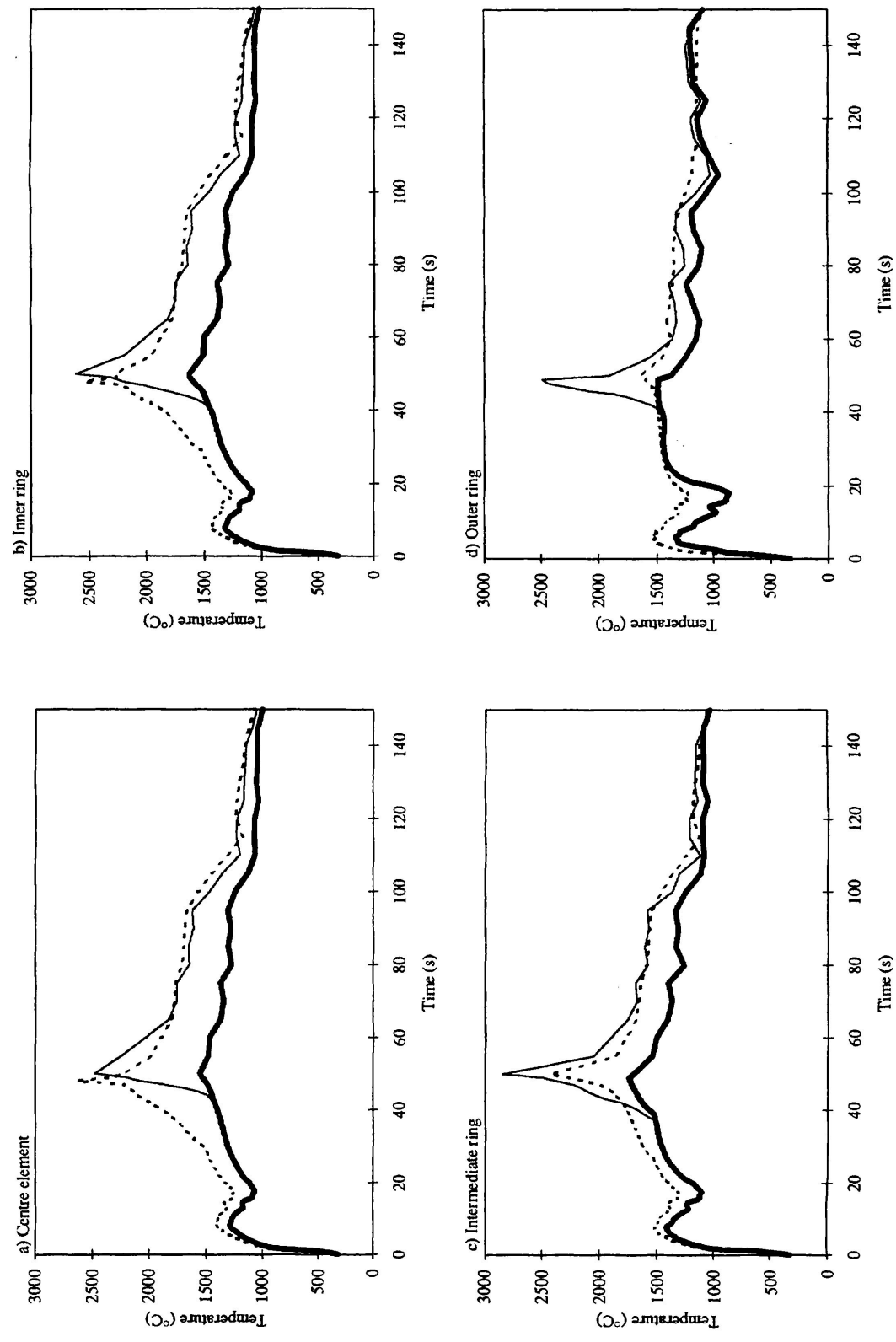

FIGURE_2.XLS/11/2/95/4:20 PM

FIGURE 3
Fuel Average Temperature at Bundle 8

Note: The severity of this transient is not typical of what is expected for large break LOCAs with ECI available.
The conditions analyzed were deliberately more severe in order to clearly indicate the effects of hfs and oxygen diffusion.

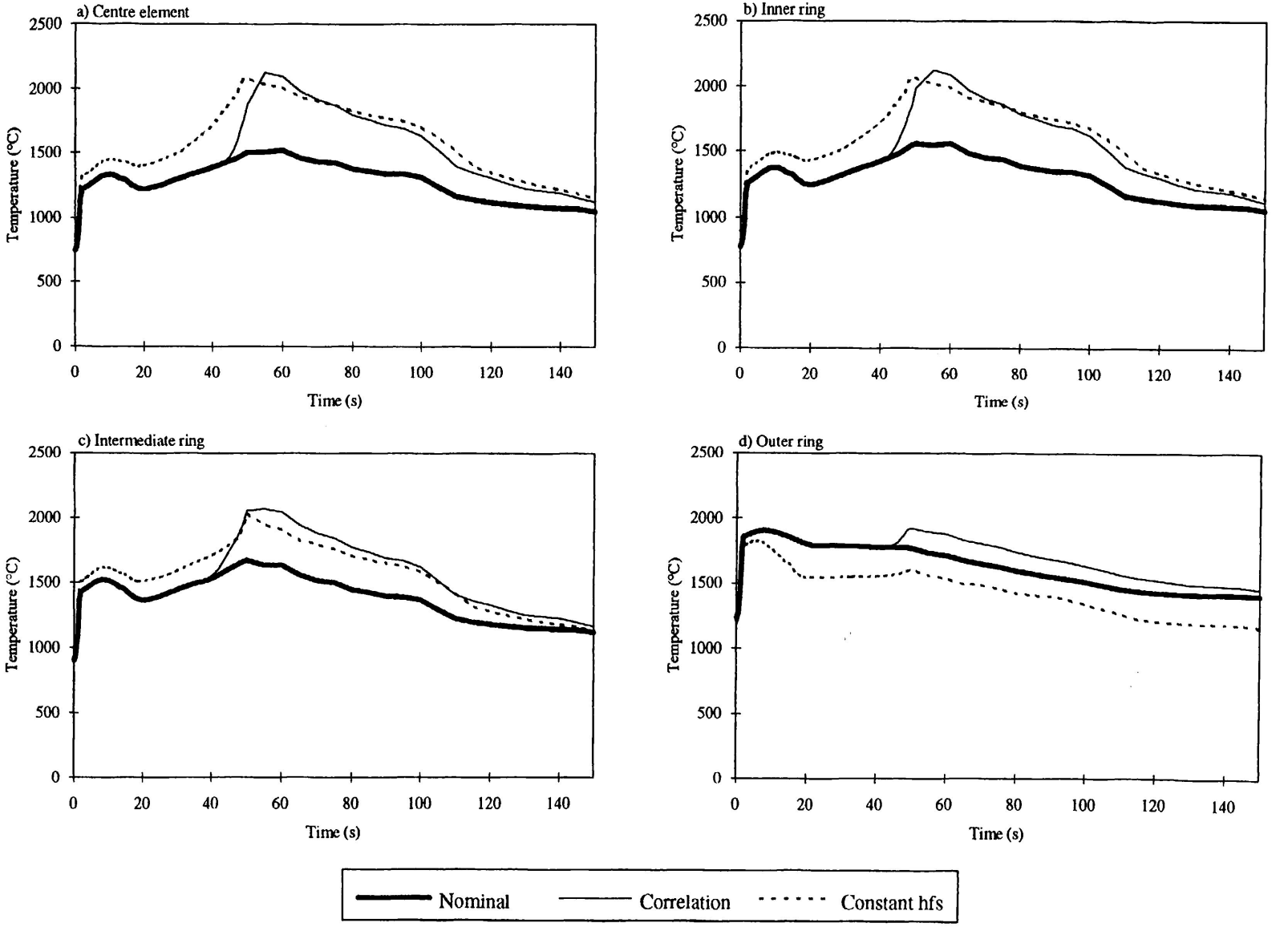

FIGURE_3.XLS/11/2/95/4:22 PM

FIGURE 4
Reacted Layer Thickness (Oxide + Alpha-Zircaloy) at Bundle 8

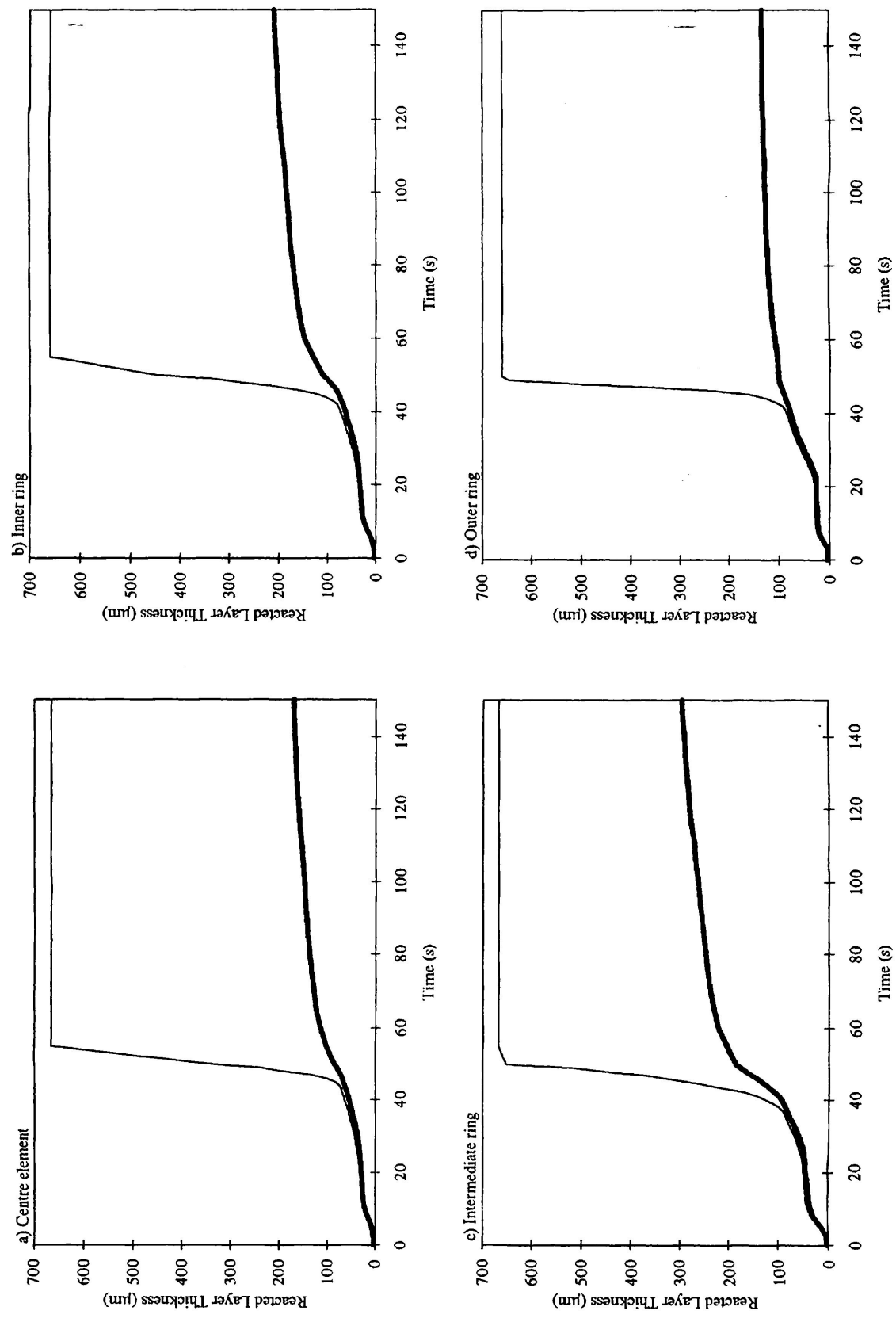

FIGURE_4.XLS/11/29/94:25 PM

FIGURE 5
Fuel-to-Sheath Heat Transfer Coefficient at Bundle 8

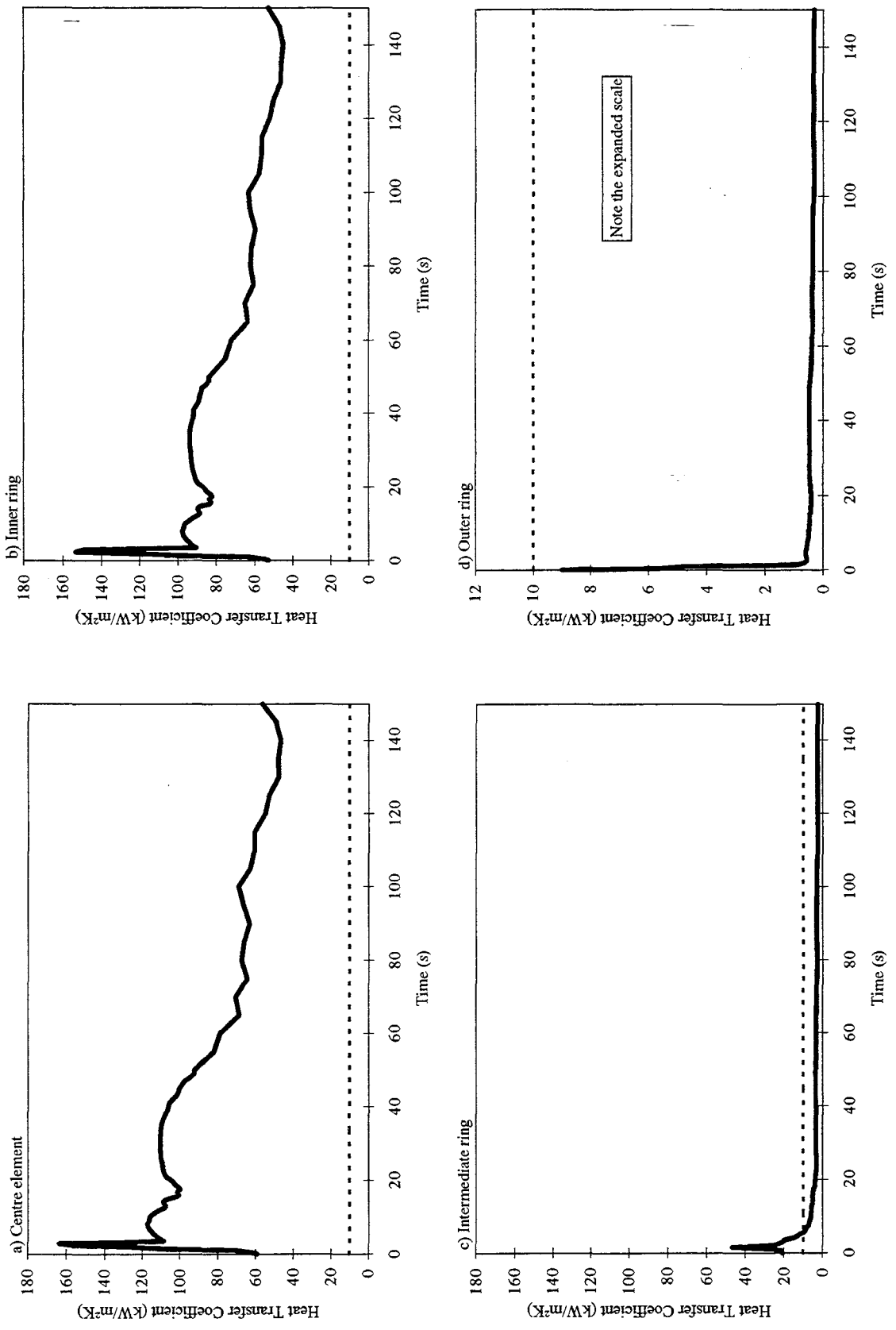

FIGURE_5.XLS/11/2/95/4:25 PM