COUPLING SUBROUTINE VERSION OF ELOCA CODE FOR HIGH-TEMPERATURE FUEL BEHAVIOUR TO CATHENA SYSTEM THERMALHYDRAULICS CODE

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ABSTRACT

This paper describes the coupling of the CATHENA two-fluid code for safety thermalhydraulics with a subroutine form of the latest version of the ELOCA code for high-temperature, thermalmechanical and fission-product release fuel behaviour. The main features of the component codes are described, followed by an outline of the thermal and geometric coupling that exists between the thermalmechanical behaviour of the fuel and the channel thermalhydraulics during a postulated LOCA. Requirements for minimum changes to the component codes and flexibility of application to other code systems, has led to an elaborate code coupling architecture, involving a number of interface routines. The code coupling methodology is described, with the main emphasis on CATHENA and ELOCA. Work done to verify the methodology is outlined. Finally, a sample CATHENA/ELOCA application is given to illustrate the potential impact of using the coupled approach in thermalhydraulic safety analyses.

1. INTRODUCTION

In traditional safety analysis, thermalhydraulic codes typically use relatively simple models for the fuel, with the main emphasis being to adequately characterize its thermal response during high-temperature transients. The more detailed assessment of fuel behaviour is carried out separately using more advanced fuel codes that model thermal as well as mechanical processes. Time-dependent thermalhydraulic boundary conditions for the advanced fuel codes are obtained from separate analyses done with the thermalhydraulic code using the simple fuel models. Thus any potential thermal and geometric feedback effects, due to the high-temperature mechanical deformation of the fuel and sheath, are not taken into account. With the increasing emphasis on best-estimate safety analysis, there is a need to perform more accurate calculations by directly accounting for feedback effects of the thermal and mechanical behaviour of the fuel on the overall thermalhydraulic and channel behaviour in a CANDU® reactor channel.

This paper describes the coupling of the CATHENA[1] two-fluid code for safety thermalhydraulics with a subroutine form of the latest version of the ELOCA code for high-temperature, thermalmechanical and fission-product release fuel behaviour.

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Requirements for minimum changes to the component codes and flexibility of application to other code systems such as CANSIM[2], which uses the ASSERT-PV subchannel thermalhydraulics code[3], has led to an elaborate code coupling architecture, involving a number of interface routines. The code coupling methodology is described, with the main emphasis on CATHENA and ELOCA. Work done to verify the methodology is outlined. Finally, a sample CATHENA/ELOCA application is given to illustrate the potential impact of using the coupled approach in thermalhydraulic safety analyses.

2. CATHENA CODE

The CATHENA (Canadian Algorithm for THErmal Hydraulic Network Analysis)[1] thermalhydraulic code was developed by Atomic Energy of Canada Limited (AECL) primarily for the analysis of postulated accident conditions in CANDU reactors. However, CATHENA is not limited to analysis of the CANDU and has been used for experimental design as well as for the design and licensing of AECL research reactors (e.g., MAPLE, NRU).

The thermalhydraulic model in CATHENA is a one-dimensional, non-equilibrium, two-fluid model, that consists of six partial differential equations for mass, momentum and energy conservation - three for each phase. The conservation equations are coupled by a flow regime-dependent set of constitutive equations defining the transport of mass, momentum and energy between the phases and between each phase and the pipe walls. In addition, the gas phase may consist of a mixture of up to four noncondensable gas components and the vapour. The code uses a staggered-mesh, one-step, semi-implicit, finite-difference method to solve the resulting set of equations. The timestep size is determined automatically by a complex timestep controller, and the timestep in not limited by the material Courant limit.

Heat transfer from and within solid surfaces (e.g., fuel and piping walls) is calculated by the GENeralized Heat Transfer Package (GENHTP), included within CATHENA. GENHTP consists of three major modelling components: 1) wall-to-fluid heat transfer, 2) wall-to-wall heat transfer, and 3) heat conduction within solids. Thermal conduction may be calculated in both the radial and circumferential directions and heat transfer between CATHENA and GENHTP is coupled in a semi-implicit manner. A user-specified number of GENHTP models can be coupled to one or more thermalhydraulic nodes. As a result, a very detailed heat transfer description of a CANDU fuel channel can be assembled by combining a number of GENHTP models. Pressure tube deformation, the zirconium-steam reaction, and radiation heat transfer may all be modelled.

CANDU fuel is modelled by a user-specified UO_2 region, gap, and fuel sheath region. Temperature-dependent properties, available within GENHTP, are generally used for the UO_2 and sheath. Although a constant gap conductance is usually used for analysis, a user-specified time-dependent value may be applied.

CATHENA also includes system models such as pressurizer, pump, valve, break discharge, ECC accumulator and separator, that are required for modelling reactor systems. An extensive control system modelling capability is also provided to model the CANDU reactor control systems (e.g., steam generator inventory and pressure regulating systems).

3. ELOCA CODE

ELOCA.Mk6, the latest release version of the ELOCA series of codes, models the transient thermalmechanical and fission-product release behaviour of a CANDU-type fuel element under high-temperature LOCA-type conditions. It has its roots with ELOCA.Mk4[4], which modelled a fuel element using a single axial segment. Subsequently, ELOCA.Mk4 was extended to handle multiple axial segments to account for axial variations in coolant boundary conditions and in metallurgical properties. Later, an improved pellet-to-sheath mechanical contact model was developed and implemented in a new interim version[5]. The FREEDOM[6] model for transient fission-gas release was incorporated into this interim version to produce ELOCA.Mk5[7-8]. Finally, several new features, including post-failure, sheath oxide-strengthening and pellet-bottoming models, and an improved interface between the ELESIM and ELOCA code, have been consolidated into ELOCA.Mk6.

The main processes modelled by ELOCA.Mk6 are:

- UO_2 pellet thermal expansion/contraction and associated crack opening. Fuel creep effects are neglected, since the main application is for fast, accident-type transients.

- Microstructure-based mechanical deformation of the Zircaloy sheath under high temperatures, including elasto-plastic pellet-to-sheath mechanical contact and oxide-strengthening effects.

- Transient, radially one-dimensional thermal conduction, accounting for radial variations in the volumetric heat generation rate due to neutron flux depression across the fuel pellet, the latent heat of UO_2 melting and of Zircaloy phase change, and the chemical heat generated in the sheath by the Zircaloy-steam reaction. The treatment of fuel-to-sheath heat transfer accounts for changes in the fuel-to-sheath gap resulting from the differential deformation of the fuel and sheath.

- Transient volatile fission-product release of the most important short-lived isotopes, including non-equilibrium growth of fission gas bubbles on grain boundaries, associated swelling, and interlinkage and venting to the element free voidage.

The initial fuel conditions for the transient are transferred from the ELESIM code[9], via a data file, called ELDAT. ELESIM simulates the thermalmechanical and fission-product release behaviour of a fuel element subjected to a specific steady-state irradiation or "power history" during NOC (Normal Operating Conditions). Parameters such as internal gas pressure, fission gas release and sheath plastic strain are important in determining the evolution of the fuel element thermalmechanical behaviour during the transient. For example, NOC operation at high linear powers to high burnups, can lead to significant fission gas release to the gap, which in turn can result in a high initial gas pressure and a low fuel-to-sheath heat transfer coefficient at the beginning of a LOCA-type transient. The high gas pressure will directly affect the extent of sheath deformation, while the low fuel-to-sheath heat transfer coefficient will directly affect the fuel heatup rate during the early stages of the transient as the coolant depressurizes.

4. COUPLED FUEL AND THERMALHYDRAULIC BEHAVIOUR

During the initial stages of a LOCA, the combination of the power pulse due to coolant voiding, and the rapid deterioration of the sheath-to-coolant heat transfer rate caused by the loss of coolant, result in sharp increases in the fuel and sheath temperatures. At sufficiently high temperatures, sheath deformation can occur, initially due to the hard contact between the thermally expanding fuel and the sheath, and subsequently due to a positive pressure difference across the sheath as the coolant depressurizes. The extent of sheath deformation due to the pressure difference will depend on the initial internal element gas pressure, which is a function of the pre-transient irradiation history, and the coolant depressurization rate.

The differential mechanical deformation of the fuel and sheath result in significant time-variations in the fuel-to-sheath heat transfer coefficient. Its magnitude can range from a high value, when the fuel and sheath are in hard contact, to a very low value, if the pressure-driven sheath deformation is high enough to result in a finite gap between the fuel and sheath.

The time-variation of the gap heat transfer coefficient directly affects the fuel and sheath heatup rates and indirectly, the coolant temperature, via the sheath-to-coolant heat transfer rate. The extent of pressure tube heatup and deformation are in turn functions of both coolant and sheath temperatures. Coolant temperatures affect the convective heat transfer rate to the pressure tube, while sheath temperatures affect the radiative heat transfer rate.

If sheath strain is significant, changes in subchannel flow areas can lead to flow bypassing and redistribution and, therefore, can also play a role in fuel and pressure tube thermalmechanical behaviour.

The above clearly shows the importance of the mechanical deformation aspects of fuel behaviour on not only the thermal response of the fuel but also its effect on channel thermalhydraulics and pressure tube thermalmechanical behaviour. Because the ELOCA.Mk6 code models the key thermalmechanical processes of a fuel element, the decision was made to couple a subroutine version of it to the CATHENA code.

At the start of this development, the release version of ELOCA.Mk6 was limited to a radially one-dimensional treatment of heat conduction in the fuel and sheath, while the CATHENA fuel model can treat both one-dimensional radial and two-dimensional radial-circumferential heat conduction. Hence it was decided that the CATHENA-ELOCA coupling should be designed to operate in two modes.

In the first mode of operation, variations in boundary conditions around the sheath are assumed to be sufficiently small that the sheath of a given fuel element or pin can be adequately represented by only one circumferential sector. The sheath sector has uniform boundary conditions comprising the sheath-to-coolant heat transfer coefficient, coolant temperature, radiative heat flux and coolant pressure. These boundary conditions, together with the normalized power, are passed to ELOCA, which in turn calculates the thermalmechanical response and returns to CATHENA the average surface sheath temperature. CATHENA uses this temperature to calculate the convective heat flux to the coolant and the net radiative heat flux to other surfaces.

In the second mode of operation, circumferential variations of boundary conditions are significant enough to represent the sheath of a given fuel pin with two or more circumferential sectors, each with a different set of boundary conditions. These boundary conditions are averaged over the entire circumference and passed to ELOCA. ELOCA then calculates the thermalmechanical response and returns to CATHENA the gap heat transfer coefficient. CATHENA uses this gap heat transfer coefficient with its own two-dimensional radial-circumferential thermal model to calculate the non-uniform temperature distribution in the fuel and sheath. To ensure that CATHENA correctly accounts for the effects of burnup on the heat generation within the fuel, ELOCA passes the radial distribution of the normalized, volumetric heat generation rate to CATHENA at the beginning of the transient.

5. GENERAL DESIGN SPECIFICATIONS

The detailed technical requirements for the code coupling and the subsequent design and implementation of the software were established on the basis of the following general specifications:

- To facilitate independent development and SQA (Software Quality Assurance) of the component codes, changes to them must be kept to a minimum.

- To achieve the highest degree of coupling, the call to the ELOCA fuel model must be done within a thermalhydraulic timestep, at the same location where the thermalhydraulic code normally calls its own fuel model.

- The coupling approach must be modular and sufficiently generalized to be easily adapted for use by not only CATHENA but also by the CANSIM code system[2], which is based on the ASSERT-PV code for subchannel thermalhydraulics[3].

- The overall structure must be flexible enough to accommodate different modes of operation and new features resulting from the future development of the component codes, with minor effort.

- To facilitate input file preparation by the user, specifications of ELOCA input options, ELDAT file identifications, and user-selected output parameters must be done using the input file structure of the thermalhydraulic driver.

The detailed technical requirements address the treatment of such aspects as: memory allocation for ELOCA variables for each fuel pin, pin identification, processing of ELOCA-specific input options, initialization using information from the ELDAT files, handling of boundary conditions at the beginning and end of a thermalhydraulic or macro timestep, and processing of user-specified ELOCA output at the end of a macro timestep.

A functional analysis of the general specifications and detailed technical requirements led to a highly modular, structured design in which virtually all important functions are performed by a system of interface modules or routines, as described below.

6. COUPLING METHODOLOGY

The overall coupling "architecture" is summarized in Figures 1(a) and 1(b). The diagrams illustrate both the logic flow and hierarchical structure of the interface between the CATHENA or ASSERT-PV/CANSIM thermalhydraulic driver programs and the subroutine version of ELOCA.Mk6.

As the Figures illustrate, most of the modules comprising the interface between ELOCA and each of the two thermalhydraulic drivers are the same. However, to more easily handle differences in the way each thermalhydraulic driver identifies individual fuel pins and manipulates the corresponding geometric parameters and thermalhydraulic boundary conditions, some of the modules were designed to be driver-program-specific (i.e., ELO_CAT and ELO_CATBC for CATHENA, and ELO_CAN and ELO_CANBC for CANSIM).

The ELOCA section of the CATHENA input file includes data on ELOCA options, such as the sheath oxidation model to be used; radial nodalization; axial segmentation and ELDAT file identifications. Following the processing of this data by the CATHENA input processor, the ELO_ALO routine allocates the necessary memory for each pin modelled by ELOCA. The memory is allocated as a contiguous block containing all ELOCA parameters required to uniquely characterize the thermalmechanical condition of a given fuel pin, at the beginning and end of a macro timestep. There is no memory allocation for fission-product release parameters; coupling of the fission-product release capability of ELOCA.Mk6 will be a future consideration.

With the MODE switch set to 0, each fuel pin modelled by ELOCA is initialized by calling the module ELO_CAT from CATHENA (or ELO_CAN from CANSIM). The module first calls ELO_PTR to identify memory location pointers for all ELOCA parameters corresponding to that pin. It then calls ELO_OPT to set the ELOCA options and linear power for the same pin. The linear power is based on the initial channel power distribution prescribed as input to the thermalhydraulic program. Lastly, it calls ELO_INT, which in turn calls ELOCA.Mk6 to read the ELDAT file corresponding to that pin. The magnitudes of the radial volumetric heat generation rates from the ELDAT file are adjusted to give the same linear power as passed from the thermalhydraulic driver, to ensure overall consistency with the prescribed channel power.

Figure 1(b) indicates that there are a number of additional initializations of local (Q_l) and global (Q_g) parameters done before control is returned back to ELO_CAT. Local parameters are those used directly by ELOCA.Mk6, whereas global parameters are those used to store the corresponding local parameters in the allocated memory for that pin. These operations are done to ensure that the global parameters for each pin are correctly initialized before proceeding to the steady-state solution.

Both steady-state and transient calculations for a thermalhydraulic macro timestep are initiated by a call to ELO_CAT from the CATHENA WALL structure, at the same point where CATHENA normally calls its own fuel model. The two solutions are specified via the MODE switch, which is set equal to 1 for a steady-state calculation and to 2 for a transient one. In both cases, the thermalhydraulic boundary conditions, comprising the sheath-to-coolant heat transfer coefficient, the coolant temperature and pressure and the radiative heat flux for one or more sectors, together with the normalized power of a given fuel pin segment, are loaded by the module ELO_CATBC.

Following the loading of the correct boundary conditions, control is passed to ELO_INT, which assigns global ELOCA parameters (Q_g) to corresponding local ones (Q_l), before calling

ELOCA.Mk6 to calculate the steady or the transient response during a macro timestep. Once this is done, newly-calculated values of local ELOCA parameters are assigned to their corresponding global ones for use in the next macro timestep.

There are a few differences in the treatment of global and local parameters in the steady-state and transient modes. Constants associated with a given pin are calculated both during the initialization and steady-state solution stages. Hence the need to save their values by assigning all local constants to their corresponding global parameters after the call to ELOCA.Mk6. During a transient, global parameters values for the beginning of the current macro timestep ($Q_{g,b}$) are set to those corresponding to the end of the previous macro timestep ($Q_{g,e}$) only if the last macro timestep was accepted.

At the end of the steady-state solution or a macro timestep during a transient, user-selected ELOCA output parameters are calculated in ELO_CALC. The CATHENA output processor calls ELO_OUT to identify their locations in memory, and subsequently writes these parameters to user-specified output files.

7. TESTING AND VERIFICATION

All interface routines, together with all modified ELOCA.Mk6 routines, were tested to ensure that they performed the intended functions. The coupled code packages were verified using test cases to confirm that the calculated results are plausible. Following is a summary of the testing and verification that was carried out.

A walk-through of all routines was performed by the coder as well as by a second party. Each line of code was checked to ensure that coding was done according to established coding practice and the routine functioned as designed.

A driver program to emulate calls from CATHENA and CANSIM, was written to test interface routines. All features of the ELOCA interface architecture were tested by stepping through the code with a debugger. The driver program was also used to establish that the subroutine version of ELOCA.Mk6 produces the same results as the original ELOCA.Mk6 program for the same input.

The memory management scheme used in the interface modules was tested using special routines designed to check discrepancies between different blocks of storage arrays. This step was taken to ensure that the storage of ELOCA variables for a given pin are not 'cross-contaminated' over several pins, and that all necessary ELOCA variables are stored and updated correctly in the interface. In particular, analogues to the interface routines ELO_INT, ELO_SET1, and ELO_SET2 were created to check that uniquely allocated ELOCA pins have exactly the same values for all storage locations when the same input options and boundary conditions are supplied.

The transfer of boundary conditions was tested by reading boundary conditions and ELOCA input options from a data file. This was done using print statements that wrote the values of boundary conditions both on the driver side, and in the interface routines.

The overall CATHENA/ELOCA and the CANSIM/ELOCA packages were verified using several verification test cases. Verification of the CATHENA/ELOCA coupling was done for both the single and multiple sheath sector modes of operation. CANSIM/ELOCA verification was done using both a radially one-dimensional, and a two-dimensional thermal calculation of a fuel pin by ELOCA. The two-dimensional feature in ELOCA was recently implemented in CANSIM but has not yet been incorporated in the CATHENA/ELOCA package.

Overall, results obtained from coupled simulations are consistent and plausible. All differences in results from uncoupled code runs can be explained in terms of the improved modelling in the coupled codes.

8. APPLICATION EXAMPLE

Here we present some results from the CATHENA/ELOCA simulation of a LOCA involving a 20% RIH (reactor inlet header) break. The emphasis is on illustrating the impact of the coupled calculation by examining some selected thermalmechanical parameters for one of the elements in the channel. More comprehensive analysis results are presented by Sabourin and Huynh in their CATHENA/ELOCA analysis of a 100% pump suction break LOCA[10].

The channel modelled contains twelve, 37-element fuel bundles, each a half-metre long. The initial channel power is 7.3 MW, with the axial flux shape being a symmetric cosine. Thus the highest linear power ratings are in the outer elements of the sixth and seventh bundles in the middle of the channel. The power histories for these bundles were chosen to be of sufficiently high burnup and linear power to result in relatively high initial values of the internal gas pressures. This was done to demonstrate the effect of significant sheath deformation on the fuel thermalmechanical behaviour during the transient.

Each pin was modelled with one axial segment, one circumferential sector and 35 radial nodes in the fuel and sheath. Symmetry was assumed about the vertical centre line bisecting the channel cross-section. This resulted in the modelling of the thermalmechanical response of 228 fuel pins by the ELOCA fuel model.

Two simulations were performed, one with CATHENA alone and the other with CATHENA/ELOCA. The CATHENA-alone simulation was done using a constant fuel-to-sheath heat transfer coefficient of 10 $kW/m^2/K$ and a uniform volumetric heat generation rate across the fuel radius.

The CATHENA/ELOCA simulation required about 25% more CPU time to run to completion. This is a relatively minor penalty in view of the more accurate and detailed calculations of the thermalmechanical fuel behaviour performed by ELOCA.

The calculated time variations of a number of key parameters for the top outer pin of the seventh bundle, are illustrated in Figures 2 to 5.

Figure 2 shows the time evolution of the engineering hoop strain, which reaches a maximum value of about 3% after 60 s. The relatively high initial internal gas pressure causes most of the sheath deformation after the first few seconds.

For this case, sheath deformation has a large effect on the fuel-to-sheath heat transfer coefficient (Figure 3), which drops from an initial value of about 20 $kW/m^2/K$ to 2 $kW/m^2/K$ after the first few seconds, when a finite fuel-to-sheath gap is formed. The coefficient continues to decrease as the gap increases with further sheath strain, reaching a value of about 0.5 $kW/m^2/K$ after 60 s.

The time variations of the fuel centreline and sheath temperatures are shown in Figure 4, which also includes the centreline fuel temperature calculated with CATHENA alone. The higher initial centreline temperature calculated with CATHENA's fuel model is due mainly to the use of a uniform volumetric heat generation rate and a lower value of the fuel-to-sheath heat transfer coefficient. The ELOCA calculation correctly accounts for the burnup-dependent effect of neutron flux depression on the volumetric heat generation rate across the pellet.

The higher centreline temperature calculated by ELOCA beyond 10 s, is a direct result of the deterioration of the fuel-to-sheath heat transfer coefficient. Higher fuel temperatures indicate lower heat transfer from the fuel to the coolant, and hence less rapid pressure tube heatup.

The more accurate pin temperature calculation with CATHENA/ELOCA leads to a better estimate of the unrestrained thermal expansion of the fuel stack (Figure 5), which is of potential use in the calculation of the overall axial expansion of the fuel string during a LOCA.

9. CONCLUDING REMARKS

A methodology has been developed to couple a subroutine version of the ELOCA code for thermalmechanical fuel behaviour, to the CATHENA system thermalhydraulics code.

The coupling approach is based on the use of a modular system of interface modules, sufficiently generalized to be easily adapted to couple ELOCA with other thermalhydraulic codes. Minor structural changes were required to couple ELOCA to the ASSERT-PV code for subchannel thermalhydraulics, via the CANSIM code system.

Extensive testing and verification was done to ensure that the individual interface modules performed as intended and that the coupled code systems produced plausible and explainable results.

A sample CATHENA/ELOCA application was presented to illustrate the potential impact of using the coupled approach in thermalhydraulic safety analysis.

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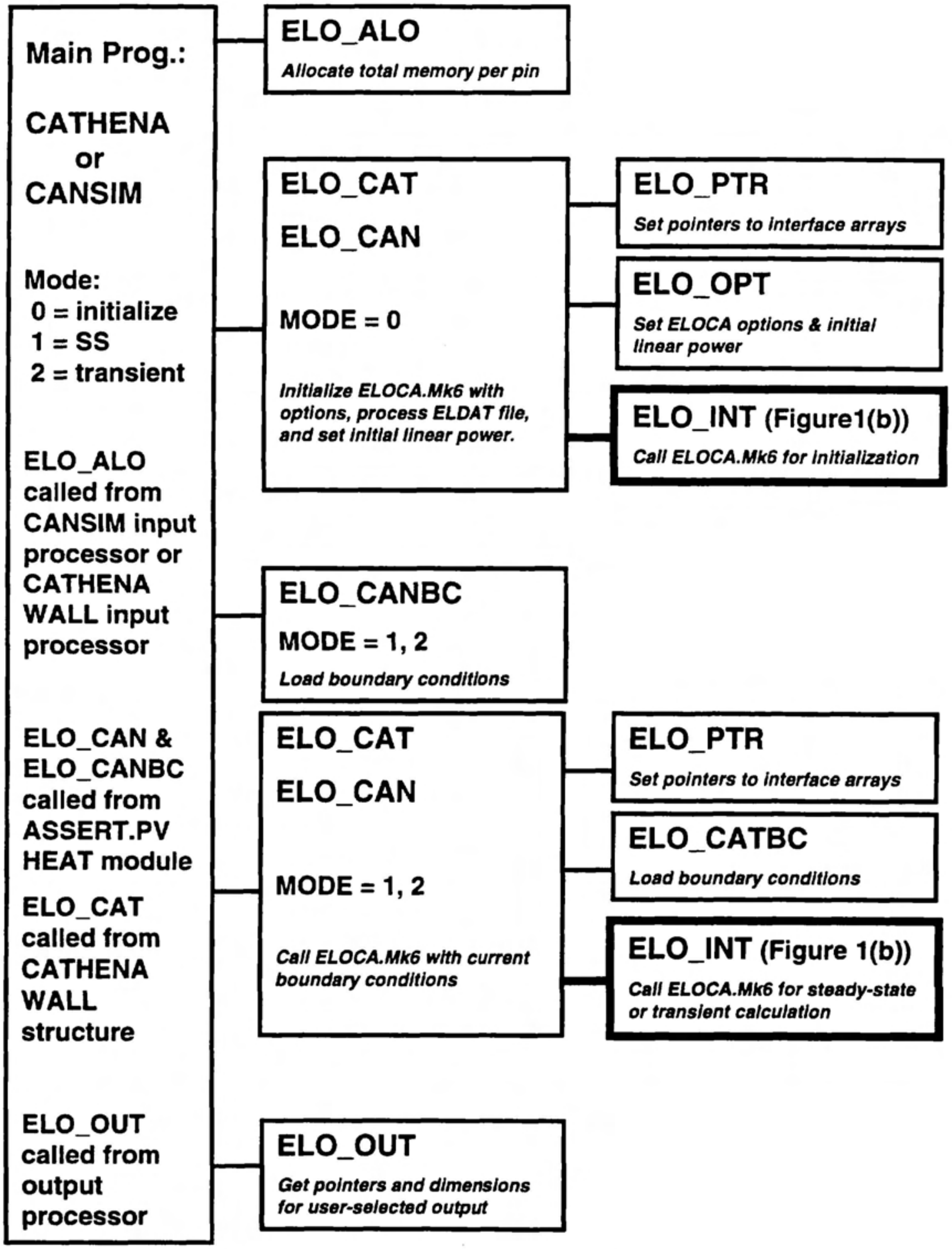

Figure 1(a): Coupling Architecture for CATHENA/ELOCA and CANSIM/ELOCA

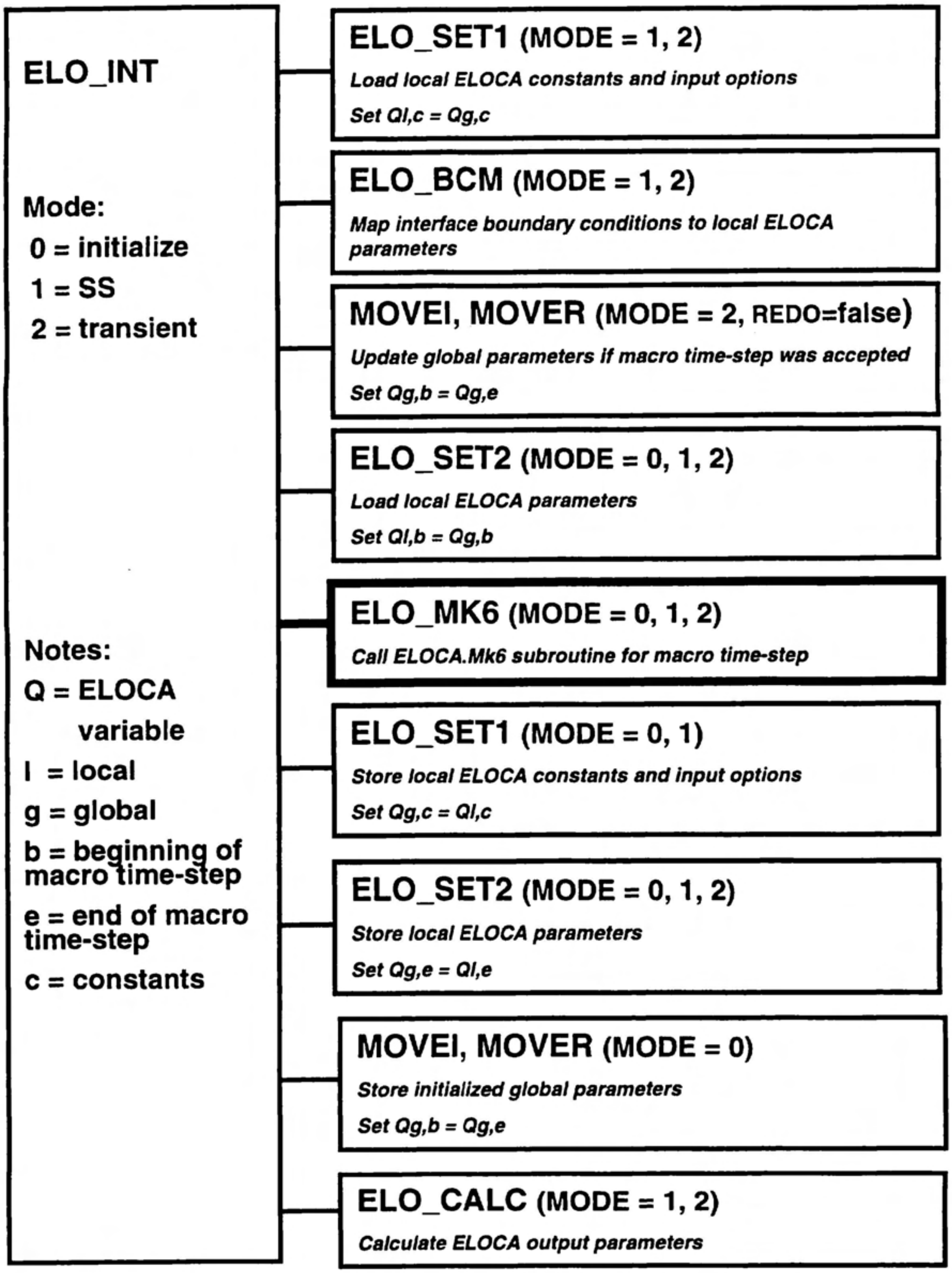

Figure 1(b): ELOCA.Mk6 Interface Architecture

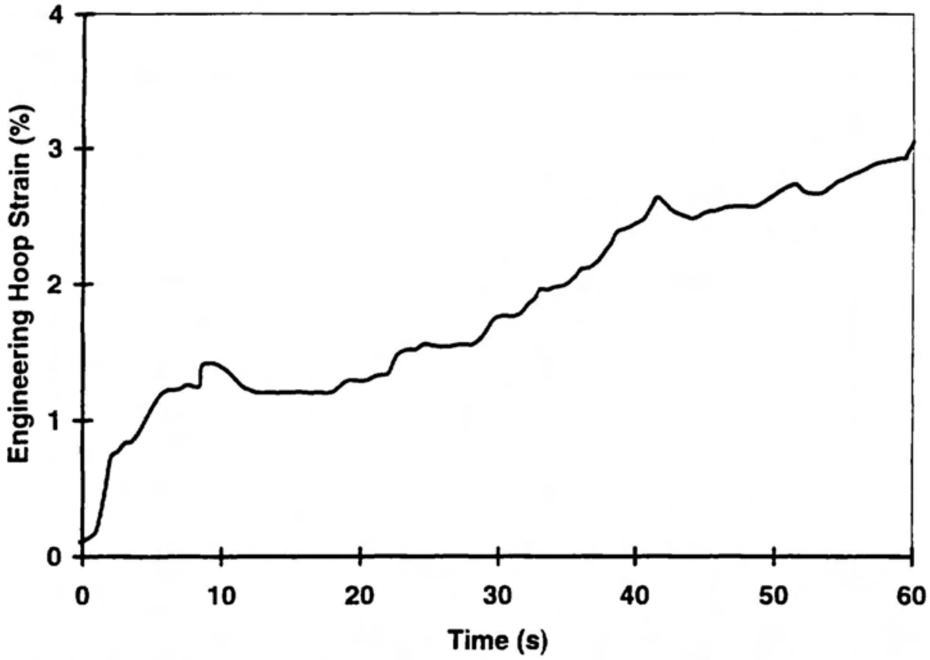

Figure 2: 20% RIH Break using CATHENA/ELOCA - Engineering Hoop Strain for Top Outer Pin of Bundle 7

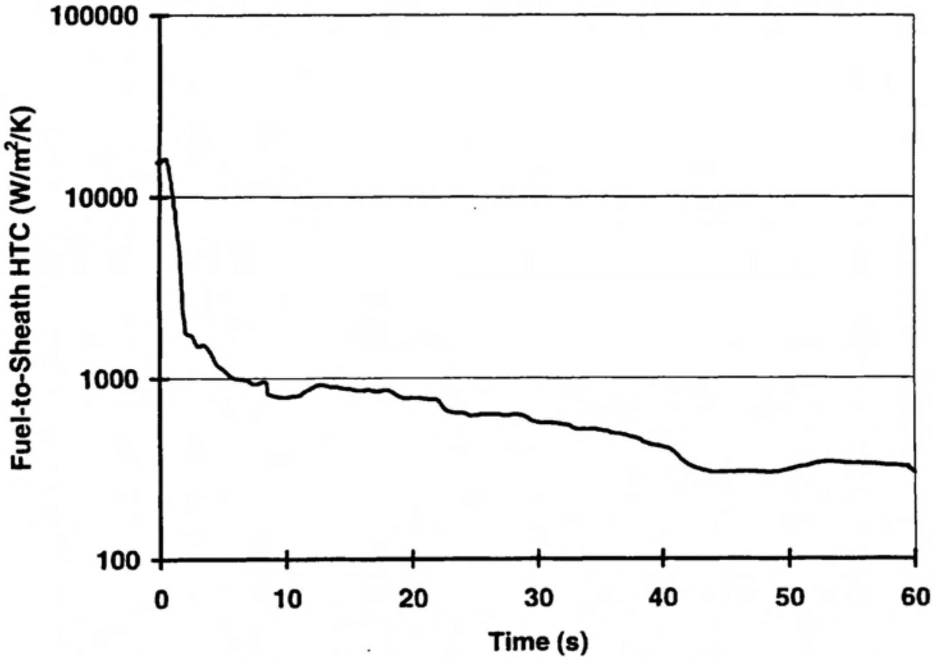

Figure 3: 20% RIH Break using CATHENA/ELOCA - Fuel-to-Sheath Heat Transfer Coefficient for Top Outer Pin of Bundle 7

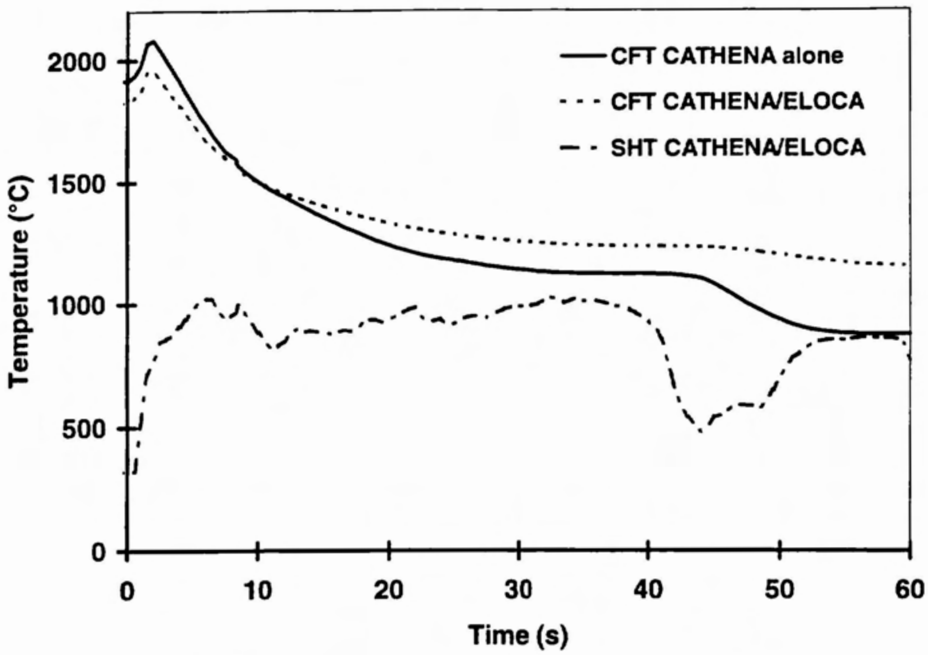

Figure 4: 20% RIH Break using CATHENA/ELOCA and CATHENA Alone - Centreline Fuel Temperature and Sheath Temperature for Top Outer Pin of Bundle 7

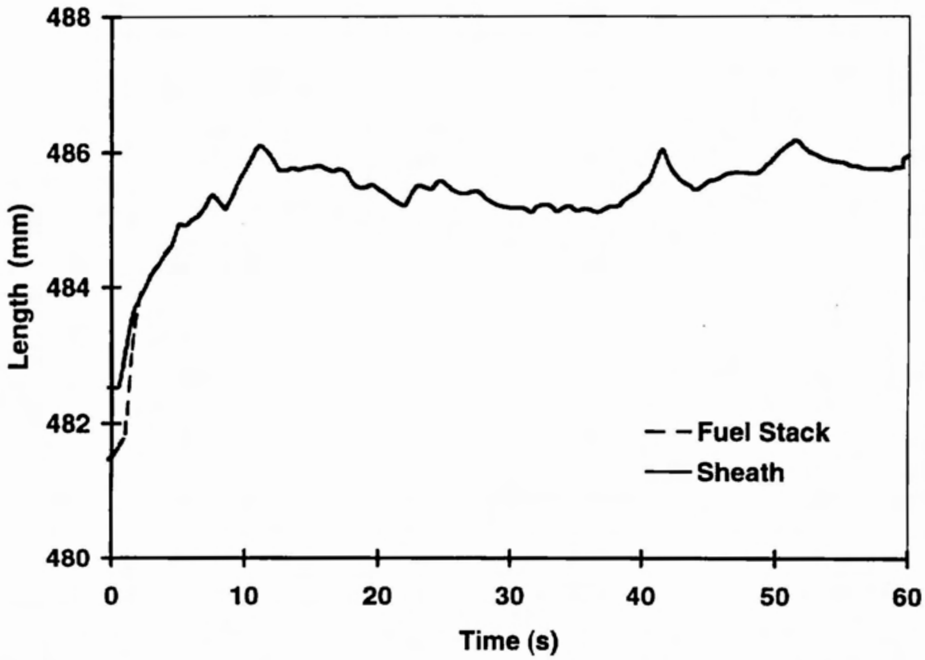

Figure 5: 20% RIH Break using CATHENA/ELOCA - Fuel Stack Length and Sheath Length for Top Outer Pin of Bundle 7