

DEVELOPMENT OF TUF-ELOCA – A SOFTWARE TOOL FOR INTEGRATED SINGLE-CHANNEL THERMAL-HYDRAULIC AND FUEL ELEMENT ANALYSES

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Abstract

The TUF-ELOCA tool couples the TUF and ELOCA codes to enable an integrated thermal-hydraulic and fuel element analysis for a single channel during transient conditions. The coupled architecture is based on TUF as the parent process controlling multiple ELOCA executions that simulate the fuel elements behaviour and is scalable to different fuel channel designs. The coupling ensures a proper feedback between the coolant conditions and fuel elements response, eliminates model duplications, and constitutes an improvement from the prediction accuracy point of view. The communication interfaces are based on PVM and allow parallelization of the fuel element simulations. Developmental testing results are presented showing realistic predictions for the fuel channel behaviour during a transient.

1 Introduction

The analysis of transient nuclear power plant response involves multiple disciplines: neutron-kinetics, thermal-hydraulics, fuel and fuel channel performance, containment and aerosol dynamic simulations. The trend is to perform such multi-discipline investigations with coupled analyses. This approach implies that many computer codes designed to simulate distinct aspects or disciplines are exchanging data during the simulation of a target scenario.

TUF-ELOCA is a tool obtained by coupling TUF [1] and ELOCA [2], and is designed to perform single channel thermal-hydraulic analyses and fuel element responses for a transient scenario. The development objectives of the new tool were:

- to provide proper feedback between the two codes, and thus providing a more integrated and realistic analysis and a better understanding of fuel channel response to a transient;
- to eliminate model duplications and conservative assumptions inherent for a non-coupled analysis, and to reduce the effort required for data transfer/manipulation, verification, and documentation;
- to develop new analysis tools as part of continuing improvement of prediction accuracy for safety analyses and for operational support analyses.

Previously, AECL had coupled CATHENA and ELOCA [3].

1.1 Coupling methodologies

The benefits of coupled analyses consist of a realistic and sound simulation of the interaction between different domains and a consistent application of different physical models by eliminating artificial assumptions, conservatism, or model duplication inherent to non-coupled analyses. This approach ensures a better understanding of the consequences of a transient with the potential for increased safety margins and represents an important step for the continuing improvement of analysis tools and methods for nuclear power plant analyses.

One of the most utilized methodologies for code to code interface is based upon **external iterations**. The methodology is used for complex analysis, and for some codes, this methodology is very well known and refined for a particular set of applications. However, the external iteration methodology is time consuming because no parallelization is possible in such an arrangement, it requires a restart capability for involved codes, the number of iterations is limited which implies a loose coupling, and preparing such coupling involves extensive user expertise.

A different coupling methodology - **integrated code** - was developed in order to solve one major issue of the external iterations method, the strength of the coupling. The integrated code methodology offers a very strong coupling between different codes, but has the disadvantage of creating large codes, with high maintenance costs and having a fixed structure with very low flexibility.

Another more flexible methodology consists of coupling existing codes in a modular code system. The **coupled codes** methodology is based on individual executables that exchange data during a transient simulation. This approach offers flexibility and is relatively easy to use, since each code in the system preserves its original input files. In addition the qualification activities can be reduced to the verification of the data exchange modules only because the algorithms of the constituent codes remain unchanged in coupled code methodology.

From a different perspective the code coupling methodologies can be seen as parallel or serial. In the first approach individual executables are running as separated processes and exchange information through virtual files or using dedicated message passing drivers such as PVM or MPI. It is then possible to utilize machines having multiple processors, or to run the coupled codes across different platforms. The degree of parallelization, however, is usually not very impressive, since time step management is required. If the serial approach is chosen for the coupled codes, the data exchange is internal and standardized interfaces can be used, for example TALINK [4]. However, the reduced modularity of such a solution is less appealing than the usage of parallel coupling based on individual executables.

One of the most important aspects for coupled codes used for transient simulations is the numeric algorithm used for time step calculations. The developers have to decide if an implicit or explicit time step algorithm is to be used. The explicit time coupling is the most commonly used method since it does not involve additional iterations between codes, and does not require further code modifications for supplementary time rejection conditions based on feedback from other codes. The common practice is for the time management to be performed by the code that requires the smallest time step during the transient. A small time step justifies the implicit algorithm and, generally, the thermal-hydraulic code is the code that uses lower time-steps and manages the transient time, the rest of the coupled applications being required to remain synchronized [5].

For all practical applications, either accident simulations, or plant operational support, the thermal-hydraulic code is the key code of a coupled analysis. As already mentioned, the thermal-hydraulic code manages the transient time, but, most importantly, the thermal-hydraulic code is responsible for the energy conservation and balance between different analyzed components, for example, between coolant, fuel bundles, and containment.

2 TUF-ELOCA Development

2.1 Description of main features

The coupled TUF-ELOCA tool was developed using two executables: TUF-PVM and ELOCA-PVM. TUF-PVM is based on TUF version 1.0.7 [1]. ELOCA-PVM is based on ELOCA-IST 2.1c [2]. Both applications can be executed in a stand-alone mode or in a coupled mode. During a coupled analysis, the execution control and information exchange is performed through the PVM version 3.4.4 driver [6]. The target platform to run these codes is Linux based. The PVM driver can work over a network, or on different computers that support this control and communication mechanism.

The architecture of a TUF-ELOCA coupled analysis is presented in Figure 1. TUF-PVM is the parent code that exchanges data with multiple ELOCA-PVM applications. A number of FORTRAN subroutines and functions, referred to collectively as the Multiple-ELOCA driver, were written to control execution of many ELOCA-PVM applications and to manage the data exchange between TUF, as the parent process, and ELOCA-PVM as children processes. The communication interfaces that are based on PVM libraries are implemented in TUF and in ELOCA in separate FORTRAN modules. These new modules are reliable and require little or no intervention from the user. Optionally, the messages exchanged between codes can be recorded and saved in special files for verification purposes.

Data are to be passed between TUF and the multiple ELOCA runs at each time step. The time step interval will be determined by TUF. The individual ELOCA runs may subdivide the time step to smaller intervals for its own calculation. The coupling is

explicit, as for each time step, TUF-PVM provides the thermal-hydraulic conditions and ELOCA-PVM children return the fuel response. For every thermal-hydraulic node, three or four ELOCA simulations are performed in order to assess the response of the entire fuel bundle to the actual environment conditions. Consequently, these calculations are performed in parallel.

The coupled codes are intended to be used for transient single channel analyses for different fuel channel designs (Bruce A and B units, Darlington, Pickering A and B units). During a coupled analysis the normal two pin representation per ring in TUF is to be replaced by a one-pin calculation. For each bundle, the fuel pin response is to be calculated for one pin representative of the pins in each ring. In other words, all pins in the same ring are assumed to be identical. There are four fuel pin rings in a 37-element bundle and three rings in a 28-element bundle. For a model of a channel containing 13 bundles of 37-element fuel bundle, 52 individual fuel pin heat transfer calculations are to be carried out. The current TUF fuel pin temperature calculation is to be replaced by an individual ELOCA-PVM run for each fuel pin modeled. The multiple ELOCA runs are independent of each other. Each ELOCA run will manage its own input and output requirements. There is no cross connection between the input run data for TUF-PVM and for the individual ELOCA-PVM runs. Data files for the ELOCA runs are managed by the driver program. Data for TUF and for the ELOCA runs are assumed to be consistent with each other.

When executed as stand-alone applications, TUF-PVM and ELOCA-PVM should be unaffected by the modifications implemented during this development. In addition, the results should be similar if these codes are executed as stand-alone applications or coupled through a PVM driver and receive the same transient input data.

If a coupled analysis is required, the analysis will start as a simple TUF analysis. TUF-PVM will launch an appropriate number of ELOCA-PVM children, control their execution, and exchange messages with these applications.

2.2 Design of TUF-ELOCA coupling

2.2.1 Multiple ELOCA Driver

The Multiple ELOCA executions driver is a set of FORTRAN modules embedded in TUF. In addition, the driver can be compiled and executed as a stand-alone application. This arrangement facilitates the development and verification activities of the ELOCA-PVM application.

The purpose of the Multiple ELOCA driver routines is to control the PVM daemon and ELOCA executions in accordance with user inputs and analysis requirements. The driver controls most of the details related to PVM implementation. Extra precautions were taken to assess the correct functioning of PVM daemon and ELOCA children. Abnormal functioning is reported in the driver main output, and, if necessary the code is stopped.

The logic flow implemented through the Multiple ELOCA driver routines consists of the following steps:

- Read the PVM Driver main input file.
- Start PVM daemon(s) on local and remote machines.
- Prepare subdirectories for each ELOCA execution. Prepare ELOCA input files.
- Start ELOCA children. Initiate communication with ELOCA children.
- For the initial steady-state step, and for any subsequent transient time steps, send the thermal-hydraulic environmental data and receive the fuel element response data for each ELOCA analysis.
- Stop ELOCA children, stop PVM daemon(s) at the end of analysis.

At end of the runs, the driver program provides a summary of the individual fuel pin results for the channel in much the same manner as is currently done in the FACTAR code.

2.2.2 TUF-PVM

For each modeled fuel pin, an independent ELOCA run is invoked via the Multiple ELOCA interface. For the bundle fuel pin calculations in the TUF code, each node modeling the reactor channel is comprised of a channel length corresponding to the fuel pin as modeled by ELOCA. An ELOCA run is carried out for one fuel pin representing all the pins in each ring of fuel pins making up the bundle. For 37 or 43-pin bundles with four rings in the bundle, four ELOCA runs are carried out. For a 28-pin bundle, three ELOCA runs are carried out in each node for the 3-ring fuel bundle configuration.

TUF provides the coolant conditions as boundary conditions to the ELOCA runs. In return, the ELOCA runs provide the fuel temperature results and the heat transfer rate from fuel to coolant. Each fuel pin is assumed to be exposed to the average mixture coolant conditions in the node. This is a simplified calculation from the “regular” modeling in TUF in which heat transfer calculations are from two representative pins for each ring. In the regular TUF model, one pin represents the pins which are exposed to the steam environment, and the other pin represents the pins exposed to two phase flow. The following boundary conditions are passed to the ELOCA runs for each thermal-hydraulic node:

- The mixture coolant average temperature based on the void fraction of the two phases,
- The coolant pressure,
- The average heat transfer coefficient,
- The radiation heat transfer rate out of the pin in each ring, and
- The fuel element relative power.

Fuel pin relative power is an optional parameter to be passed from TUF. Alternatively, the ELOCA driver program calculates the fuel pin power from neutron-kinetics power input data to be fed to ELOCA. In such case the power is fed also to TUF.

As in the current TUF code calculation for mixture flow, one heat transfer coefficient is calculated and used for all fuel pins in the bundle. The heat transfer coefficient is calculated from the coolant mixture conditions and from an average sheath temperature from all the pins in all the rings. That arrangement permits a concurrent ELOCA simulation for any given TUF node. In other words, heat transfer from fuel pins to coolant is calculated one node (or bundle) at a time. The ELOCA runs for the representative pin in all rings in a node are hence carried out in parallel. The calculations for pins in different nodes remain in sequential order, one node at a time.

The TUF radiation model from fuel pins to pressure tube and between fuel pins of different rings is retained. There are two options for the calculations. One allows only radiation between adjacent rings of fuel pins and from the outer ring to the pressure tube. The other makes use of view factors between pins in different rings and from pins to the pressure tube. There is only one set of view factors implemented in the code. The view factors matrix can be set to account for the channel geometry change after pressure tube ballooning.

Pressure tube ballooning calculations are preformed by TUF. Heat transfer to the calandria tube and to the moderator is allowed. Pressure tube straining and subsequent ballooning contact with the calandria tube are calculated.

From the ELOCA calculation for each pin, the following data are passed back to TUF:

- The heat transfer rate from the fuel pin to the coolant,
- The fuel pin centre line temperature, the fuel pin average temperature, the sheath average and sheath outer temperatures,
- The fuel pin radius, the sheath outside radius,
- The hydrogen generation rate.

The heat transfer rate is not a native parameter in ELOCA. It is calculated in the ELOCA-PVM driver program and is equal to the TUF heat transfer coefficient multiplied by the difference between the sheath outside temperature (from ELOCA) and coolant temperature (from TUF) and the ELOCA sheath outside area.

The hydrogen generation rate is used in TUF only if the TUF non-condensable gas option is invoked.

The following additional changes have been made to TUF to facilitate data handling:

1. An option has been added to the code to read in the RFSP power data, the time relative power of the bundle in each node. At present, the option is only partially

implemented without the “log” power interpolation as normally employed for power generation data for FACTAR/ELOCA.

2. Channel power is calculated backwards from the bundle power if power is from the relative power from RFSP power data or from ELOCA.
3. Code changes were executed in TUF to maintain and to account for the different sheath radius and fuel pellet radius from ELOCA for pins of different rings in a node for the node heat transfer calculation in TUF.
4. An option has been added to allow the TUF channel flow geometry to change in accordance with the fuel sheath radius from ELOCA. An option has also been added to include the pressure tube geometry change due to strain and ballooning of the pressure tube. The geometry parameters modified are the bundle heat transfer area, the coolant flow area, the flow hydraulic diameter, the volume of the node, the inner radius of the pressure tube, and the heat transfer area between pressure tube and coolant. Changes in the pressure tube thickness and outside radius are already included as part of the strain calculation.

2.2.3 ELOCA-PVM

New functionality and related variables implemented in ELOCA-IST 2.1c to create a PVM interface for coupling with TUF were encapsulated in a FORTRAN module. This module separates PVM related data, subroutines and functions from the ELOCA original algorithm.

The following functions are performed by the interface module:

- Detect if ELOCA-PVM is executed standalone or remotely.
- Manage the data transfer between parent application and the current child process.
- Prepare transmitted data (using ELOCA variables).
- Detect abnormalities or errors related to PVM daemon performance and data broadcasting.
- Report transferred data and other details related to interaction between the child application and the PVM daemon.

From the interface perspective, the content and the structure of modeling data is of interest. A child ELOCA-PVM exchanges data packages with the parent process. The data transfer is performed through the PVM daemon. The data communication protocol implemented in ELOCA-PVM is based on a simple rule. The child is listening to and replies on each data package received from the parent. This rule ensures a reliable data exchange between both applications and establishes the required hierarchy based on the parent as the initiator of the communications and the child as the application that responds to parent requirements. At the beginning of ELOCA-PVM execution initialization data packages are exchanged to initiate and confirm the parent/child relation.

3 Testing TUF-ELOCA coupling

As the TUF and ELOCA codes have been independently validated, the qualification of the coupled TUF-ELOCA version will focus on the correctness and accuracy of the implementation. To that end, a number of simulations have been executed with the coupled version of TUF-ELOCA. For these test cases the data exchanged between TUF-PVM and ELOCA-PVM was verified for correctness. The verification activities are facilitated by the modular design of the coupled tool and by the fact that these applications can be executed in stand-alone mode.

A comparison of fuel and pressure tube temperature predictions is made for Darlington NGS Channel T16 between two analyses for the same transient conditions. The first analysis consisted of a stand alone TUF simulation using the internal fuel model, followed by a FACTAR [7] analysis with input from TUF. A second analysis was performed using the coupled TUF-ELOCA. Figures 2 – 4 show comparison plots for the following parameters for the first 30 seconds of a stylized LBLOCA case:

- Bundle 6 - Outer Ring Fuel Centre-Line Temperature
- Bundle 6 - Outer Ring Outer Sheath temperature
- Bundle 6 - Pressure Tube Temperature

The results show an overall consistency between TUF, FACTAR and TUF-ELOCA. The TUF-ELOCA predictions and FACTAR predictions for the centerline temperature are in good agreement. The overall trend of the sheath temperatures for the outside ring of bundle number 6 shows that TUF-ELOCA predicts slightly higher temperature at the end of the transient. Both codes predicted the same peak values for the sheath temperature.

The peak temperature for the pressure tube wall presents the same results for all three simulations, TUF stand-alone, FACTAR and TUF-ELOCA. As well, the pressure tube ballooning time is in good agreement between simulations showing consistent models in TUF and FACTAR.

During the LBLOCA analyses the CPU times for TUF-PVM and for the 52 or 48 ELOCA-PVM children were monitored. Comparing the total of the CPU times with the elapsed time a maximum parallelization factor of 2 was obtained when the coupled analysis is executed on a computer having 4 processors. The parallelization factor decreases when the applications are executed on different computers. This is caused by the time necessary to broadcast large amounts of data through the network between the parent and children applications.

Similar results were obtained for transient analyses performed for Pickering B and Bruce B single channel transient analyses. For those cases, the coupled TUF-ELOCA show slightly lower results for the peak and overall sheath temperatures.

The coupled TUF-ELOCA has also been used to model a Loss of Reactivity Control (LORC) event. The objective of that analysis is to calculate the dry-out time and UO₂ centerline melting time for a specified reactivity insertion rate. The TUF-ELOCA tool predicted realistic behaviour of fuel channel/fuel bundles transients during such transients.

4 Conclusions

The TUF-ELOCA tool has been developed in order to improve the prediction capabilities for single channel transient analyses. By having a detailed fuel element response analysis linked with the thermal-hydraulic analysis, the new tool offers more realistic predictions for safety or for operational support analyses. The original algorithms of TUF and ELOCA were not modified, and as a result the independent validation for TUF, or for ELOCA, is still applicable for the coupled analysis.

The coupled tool is developed based on a modular design, and is using modern execution control and data messaging techniques based on PVM driver. The modular design ensures independent maintenance and development for TUF or ELOCA and is scalable to different fuel channel designs. In addition the modular design assures a proper use of computing resources taking advantages of parallel computing.

The implementation details for the PVM interfaces in TUF and in ELOCA were encapsulated in specific modules and are not transparent to the users. The coupled application is easy to use and preserves the original input/output files specific to stand-alone TUF and ELOCA.

The tool was tested for LBLOCA and LORC accident scenarios considering 37 or 28-elements fuel bundles. Developmental testing show realistic values predicted for the highest sheath and pellet temperatures.

5 Acknowledgments

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6 Acronyms

AECL	Atomic Energy of Canada Limited
COG	CANDU Owner Group
ELOCA	Element Loss Of Coolant Analysis
FACTAR	Fuel And Channel Temperature And Response

LBLOCA	Large Break Loss of Coolant Accident
LORC	Loss of Reactivity Control
MPI	Message Passing Interface
PVM	Parallel Virtual Machine
TH	Thermal-hydraulic
TUF	Two Unequal Fluids

7 References

- [1] W.S. Liu, R.K. Leung, J.C. Luxat, "Overview of TUF Code for CANDU Reactors", Fifth International Conference on Simulation Methods in Nuclear Engineering, Montreal, Canada, September 8-11, 1996.
- [2] A.F. Williams, "The ELOCA Fuel Modelling Code: Past, Present and Future", Presented at the CNS 9th CANDU Fuel Conference, September 18-21, 2005.
- [3] L.N. Carlucci, J.R. Gauld, D.J. Richards, V.I. Arimescu, "Coupling Subroutine Version of ELOCA Code for High-Temperature Fuel Behaviour to CATHENA System Thermalhydraulics Code", Fifth International Conference on Simulation Methods in Nuclear Engineering, Montreal, Canada, September 8-11, 1996.
- [4] L. Ammirabile, S. Walker, "Large-Break LOCA Studies: Computational Analysis of Clad Ballooning and Thermohydraulics in a PWR", International Conference Nuclear Energy for New Europe 2002, Kranjska Gora, Slovenia, September 9-12, 2002.
- [5] D. Grgic, "Basis for Coupling 3D Neutron-Kinetics/Thermal-Hydraulics Codes", 5th Seminar and Training on Scaling, Uncertainty and 3D Coupled Calculations in Nuclear Technology, 3DS.UN.COP 2006, Barcelona, Spain, January 23 – February 10, 2006.
- [6] Al Geist, et al., "PVM: Parallel Virtual Machine - A Users' Guide and Tutorial for Networked Parallel Computing", MIT Press, Massachusetts, USA, 1994.
- [7] C.J. Westbye, R.C.K. Rock, L. Sie, G.R. Berzins, "Validation of FACTAR 2.0 Against Small Out-of-pile Laboratory Tests", 7th International CNS CANDU Fuel Conference, Kingston, Ontario, September 23-27, 2001.

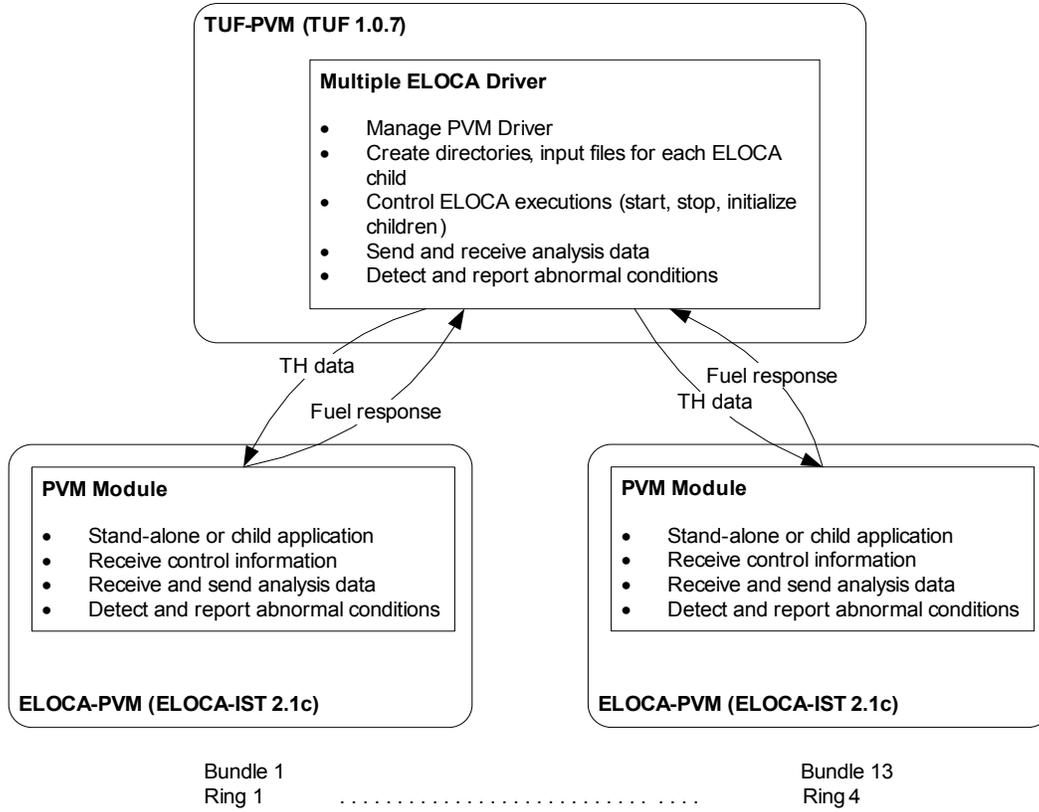


Figure 1. Architecture of TUF-ELOCA coupled analysis

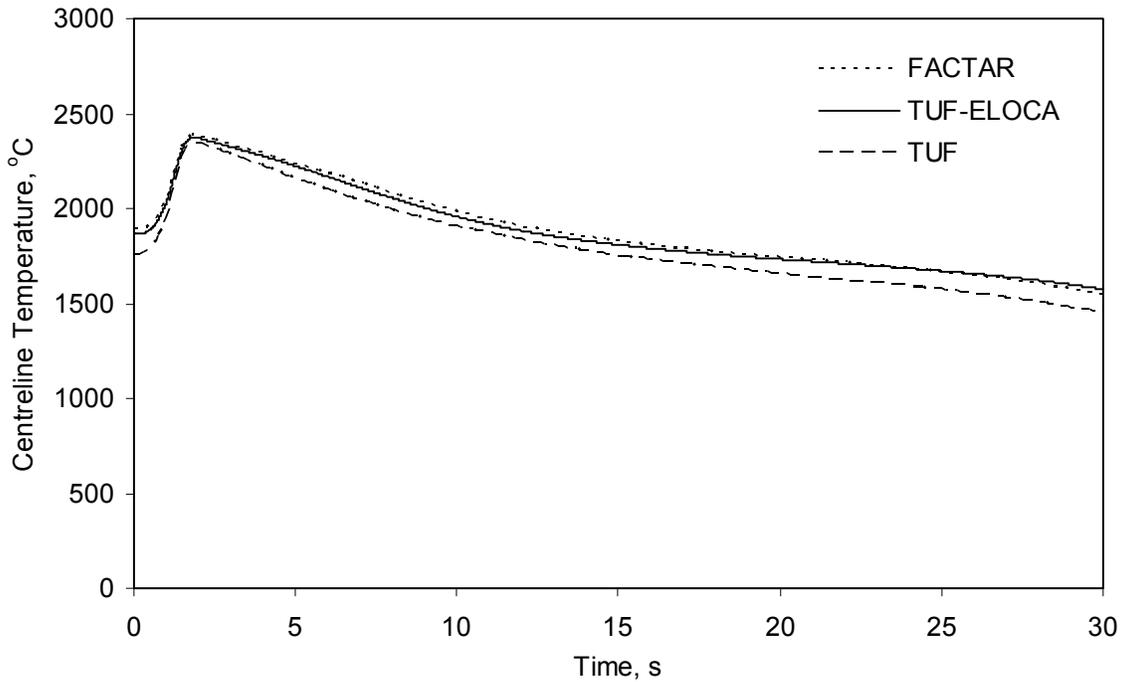


Figure 2. Darlington single channel transient - Bundle 6 - Outer Ring Fuel Centre-Line Temperature

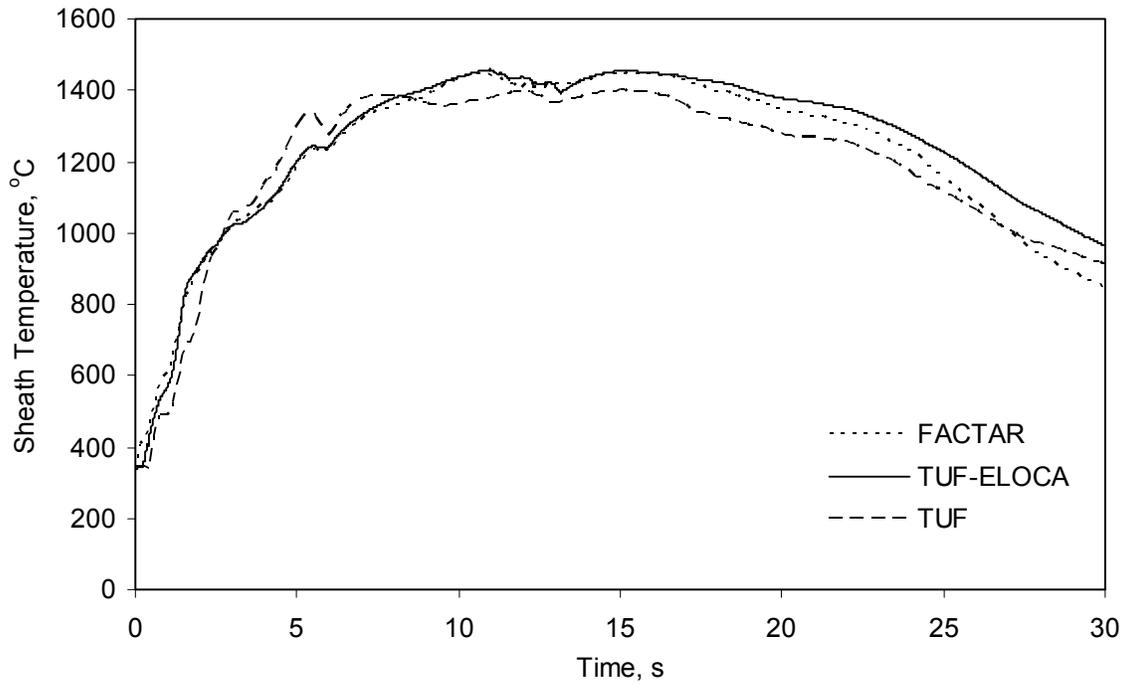


Figure 3. Darlington single channel transient - Bundle 6 - Outer Ring Sheath Temperature

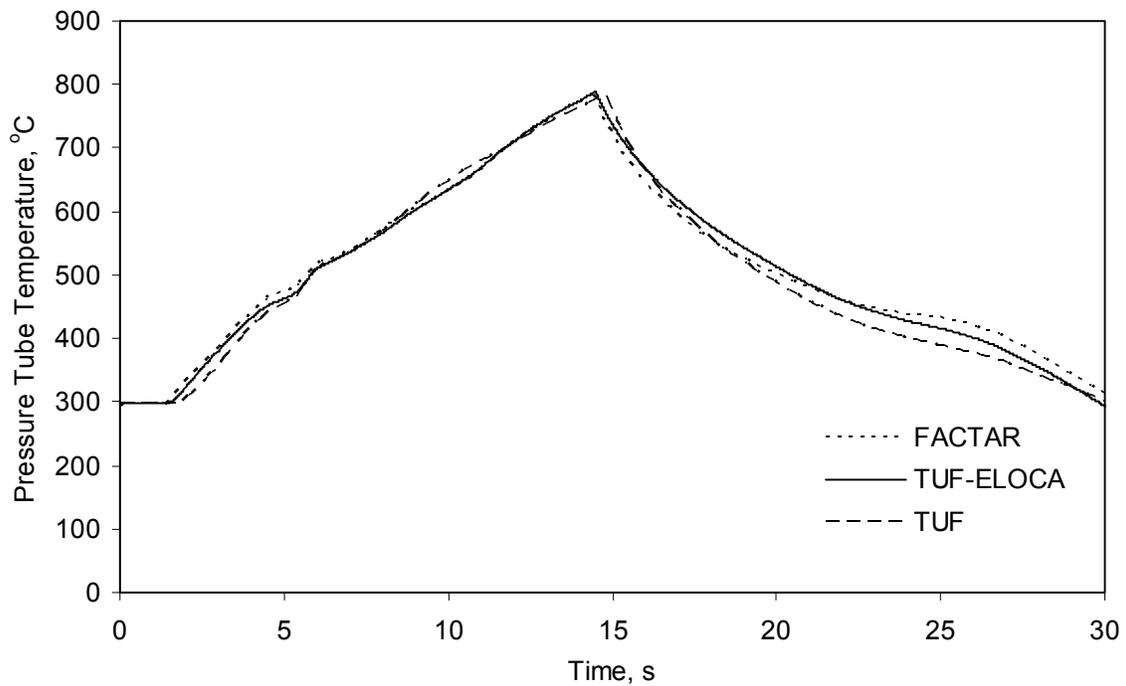


Figure 4. Darlington single channel transient - Bundle 6 - Pressure Tube Temperature