THE FUEL AND CHANNEL THERMAL/MECHANICAL BEHAVIOUR CODE FACTAR 2.0 (LOCA)

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ABSTRACT

The computer code FACTAR 2.0 (LOCA) models the thermal and mechanical response of components within a single CANDU fuel channel under loss-of-coolant accident conditions. This code version is the successor to the FACTAR 1.x code series, and features many modelling enhancements over its predecessor. In particular, the thermal hydraulic treatment has been extended to model reverse and bi-directional coolant flow, and the axial variation in coolant flow rate. Thermal radiation is calculated by a detailed surface-to-surface model, and the ability to represent a greater range of geometries (including experimental configurations employed in code validation) has been implemented. Details of these new code treatments are described in this paper.

1. INTRODUCTION

The computer code FACTAR (Fuel And Channel Temperature And Response) models the thermal and mechanical behaviour of a single fuel channel under loss-of-coolant accident (LOCA) conditions. The code version FACTAR 2.0 is the successor to the FACTAR 1.x code series[1] (FACTAR 1.x generically includes the code versions FACTAR 1.0 through FACTAR 1.3.1). The code version FACTAR 2.0, as discussed in Reference 1, was originally intended to model high-temperature phenomena applicable to a postulated large break LOCA with loss of emergency coolant injection scenario. The released FACTAR 2.0 version does not have many of these models in place, although coding structure and development methodology allows for them to be readily integrated in the future. To distinguish the code which is the subject of this paper from that discussed in Reference 1, the current version is referred to as FACTAR 2.0 (LOCA), implying that it is applicable to large break LOCA scenarios with emergency coolant injection available.

FACTAR 2.0 (LOCA) represents a significant departure from earlier code versions. Primarily, this code has been developed to incorporate more rigorous constituent models and therefore establish a strong foundation for more challenging applications. Among many improvements, FACTAR 2.0 (LOCA) provides stronger numerical coupling between the thermal hydraulic and fuel solutions, a better representation of fuel channel thermal hydraulic boundary conditions, more flexibility in the types of geometries that can be represented and more internal checks to ensure the correctness of results.

Fuel element temperature and mechanical response is still calculated using the ELOCA[2,3] code. Convective boundary conditions for the fuel element calculation are provided by the thermal hydraulic solution (performed by treating the coolant as a homogeneous mixture), including the effect of reverse and bi-directional coolant flow. The axial coolant flow rate variation due to phase change and transient effects is also explicitly modelled. Channel boundary conditions required for this calculation are input by the user and are typically obtained from a system thermal hydraulic code. Convective heat transfer coefficients are calculated through a range of correlations providing a detailed representation of the boiling curve. Thermal radiation, another boundary condition for the fuel element calculation, is calculated using a high resolution circumferentially segmented surface-to-surface treatment similar to that employed in the codes HOTSPOT[4] and SMARTT[5]. Pressure tube and calandria tube thermal/mechanical behaviour (*i.e.*, heatup and strain) are calculated using the solution of the one-dimensional transient energy equation and the strain model of Shewfelt[6].

This paper discusses the models implemented in FACTAR 2.0 (LOCA) and the range of applicability of the code. Particular emphasis is placed on the improvements made in modelling compared to earlier code releases.

2. OVERVIEW

FACTAR represents the thermal and mechanical behaviour of components within a single fuel channel under loss-of-coolant accident conditions, including the UO_2 fuel, Zircaloy sheath, pressure tube and calandria tube. FACTAR 1.0 was the first released code version, and coupled a relatively simple thermal hydraulic treatment with the sophisticated fuel code ELOCA; its basis was the CANSIM-PLE[7] code. The basis of this thermal hydraulic treatment was a homogeneous two-phase flow model with uni-directional flow throughout the transient; the coolant flow rate and pressure was constant along the fuel channel during each time step, but could vary with time. This treatment was sufficiently accurate to provide the necessary boundary conditions to the fuel solution[8]: convective heat transfer coefficients, convective sink temperature, coolant pressure and thermal radiation heat fluxes. In turn, the fuel portion of the code (ELOCA) returned sheath strain and surface convective heat flux, used to update the flow area and coolant temperature. In later versions of the FACTAR 1.x code family (FACTAR 1.2 and 1.3), the thermal hydraulic treatment was strengthened but the basic assumptions (uni-directional flow, axially-invariant flow rate) remained.

In FACTAR 2.0 (LOCA) these assumptions have been removed. Forward, reverse and bi-directional flow are all explicitly modelled; the flow direction is specified at each time step as a boundary condition from a system thermal hydraulic code. The mass conservation equation is solved to obtain the axial variation in flow rate at each time step. The communication between the fuel model and thermal hydraulic model has remained relatively unchanged, but the order of calculations revised to yield stronger numerical consistency. The following sections provide an overview of the calculational sequence of the code, highlighting the modelling improvements over the FACTAR 1.x code series. A flowchart of the main calculational steps is given in Figure 1.

2.1 Initial and Boundary Conditions

FACTAR 2.0 (LOCA) requires a number of initial and boundary conditions in order to perform its calculation. The initial fuel conditions (such as fuel porosity, initial radii, radial heat generation distribution, *etc.*) are obtained from FACTAR_SS[9], a multi-element driver for ELESIM-II (MOD 10)[10].

Boundary conditions, required throughout the transient, consist of normalized thermal power, coolant pressure, inlet coolant enthalpy and inlet coolant flow rate.

Power information can be specified in one of three ways: (i) a single normalized overpower transient, which is applied to each modelled pin in the channel; (ii) a specific normalized overpower transient applied to each axial segment (bundle); or (iii) sufficient information can be specified to allow the code to

calculate an axially varying overpower transient. Options (i) and (iii) were available in FACTAR 1.x; option (ii) has been added to FACTAR 2.0 (LOCA) to allow greater flexibility in specifying power boundary conditions. The information required for the third option includes axial power distributions at zero and at five seconds, axial energy deposition profiles over the first five seconds and a nominal power shape that is scaled for consistency with the energy deposition. The advantage of this latter method is that it allows analysts to combine neutronic data from distinct fuel channels (*e.g.*, the channel with the highest energy deposition in the fuel with the channel with the most peaked axial profile). This calculation is described in more detail in Reference 11.

Thermal hydraulic boundary conditions are channel pressure, inlet channel flow rate and inlet coolant enthalpy. The specified pressure is applied at all axial locations along the channel at each time step (used for coolant property evaluation and as a component in the sheath and pressure tube strain calculations). The solution for fuel channel characteristics, as in previous code versions, is done in one pass using calculated outlet quantities at a given axial location as inlet conditions for the next downstream bundle. Variations in flow direction are specified through the inlet flow transient. If a positive flow rate is specified, the coolant flow and enthalpy boundary conditions are applied at the entrance to the bundle closest to the channel inlet under normal operating conditions ("bundle 1") and calculations proceed downstream in the same direction as coolant flow under nominal conditions. If a negative flow rate is specified, the coolant flow is taken in the reverse direction from nominal; the boundary conditions are applied at the outlet of the last bundle in the channel under normal operating conditions, and calculations proceed in the opposite direction. Bi-directional flow can also be modelled, by specifying the location of a "virtual inlet" within the fuel channel. This virtual inlet can be located at the junction between any two bundles; in this case, calculations are segregated between the stagnation point and the nominal inlet (where the local flow is in the reverse direction), and between the stagnation point and the nominal outlet (where the local flow is in the forward direction).

FACTAR 2.0 (LOCA) solves both the mass and energy conservation equations within each axial segment at each time step. The boundary conditions appplied are typically generated by system thermal hydraulic codes which include conservation of momentum in their system equations (*e.g.*, TUF[12]). The boundary conditions applied in a FACTAR simulation are constantly refreshed with the system thermal hydraulic code predictions throughout the transient. As such, FACTAR calculates local thermal hydraulic transients (such as coolant enthalpy and mass flow rate) within a channel that agree very well with the system thermal hydraulic code predictions. Utility codes have been created to prepare the flow transient for input to FACTAR.

The code FACTAR 2.0 (LOCA) has been structured on the basis of a generalized geometry. The ability to define the modelled geometry solely through input data represents a significant departure of FACTAR 2.0 (LOCA) from earlier code versions and is described in detail in the next section.

2.2 Generalized Geometry

The "generalized geometry" model serves to separate the solution of the physics, contained in the code, from the geometry, specified in separate input files. The code has the ability to represent any geometry comprised of cylindrical fuel elements contained within at least one cylindrical tube (*e.g.*, a pressure tube). Any distribution of fuel elements within the cylindrical tube is possible; the spatial distribution of pins is only required to determine the thermal radiation view factor matrix for that particular geometry. The geometrical specification gives the code the ability to model, for example, single element or trefoil geometries with no modifications to the code. This ability greatly simplifies code validation, since the same executable is used for validation exercises and analysis runs.

The generalized geometry model requires a number of parameters to represent and characterise the bundle and channel: physical dimensions of the pins and tubes, surface emissivities, radial and circumferential nodalization information are among the most basic. Figure 2 shows a possible representation of a 37-element bundle for use in FACTAR 2.0 (LOCA) which makes use of symmetry; two 1/12th symmetric

wedges are shown, along with a sample sectorization for each fuel pin. Each pin falling partially within the 1/12th wedge would be modelled explicitly; in this case five representative elements are considered. More detailed information required to define the geometry includes "contact models". These specify what each surface within the model are in contact with. The fuel elements and pressure tube/calandria tube can be discretized into an arbitrary number of circumferential sectors. Each sector can, in general, be in contact with a different "coolant flow channel" (defined below) or another solid surface. As part of the generalized geometry representation, each bundle in the channel is defined to have an initial "state", where the state is defined by the information previously described. Gross geometry deformations can then be modelled simply by allowing transitions between states under pre-determined conditions. In FACTAR 2.0 (LOCA), state transitions from the "nominal" geometry to a geometry in which the pressure tube has ballooned is supported (note, however, that the continuous increase in pressure tube diameter is modelled within the nominal state). Future code versions will support a number of state transitions, for example high temperature bundle slumping, pressure tube sagging or eccentric bundle states. The geometry specification has been designed to include some information that is not actively used in the current version (such as surface-surface contact), but will be used in later releases intended for more challenging applications, such as a loss-of-coolant accident with coincident loss of emergency coolant injection (LOECI) scenarios.

The flow cross section can be divided into any representation of coolant flow channels desired by the user; the only information required by FACTAR is the relative flow areas (fraction of the total cross-sectional flow area) and contact information (required to assess convective energy deposition/removal with the coolant and change in flow area due to strain of pins and pressure tube). Each cross-sectionally *segregated portion of* coolant is referred to as a "flow channel". These coolant flow channels may be bounded by a physical surface (such as a portion of a fuel sheath or the pressure tube), or may be bounded by any construction line drawn within the bundle. In FACTAR 1.x, the coolant representation was limited to a flow annulus model: coolant bounded by adjacent fuel rings (or the outermost fuel ring and the pressure tube) were considered to be distinct flow annuli (with this definition, both 28- and 37-element bundles consist of four flow annuli). How the convective heat transfer was partitioned to each flow annuli depended on the user-selected mixing model; options included treating all flow annuli as well-mixed along the length of the bundle ("FACTAR total mixing", reducing the four annuli to a single flow channel), or treating all flow annuli distinctly along the bundle but mixing the coolant at the bundle outlet ("CHAN total mixing"). Investigations of coolant mixing in a fuel channel are currently underway[13] to determine the mixing model which best represents the physics within a CANDU fuel bundle for various flow conditions.

The generalized "flow channel" representation in FACTAR 2.0 (LOCA) can be set up to mimic all of the mixing options available in FACTAR 1.x. Coolant mixing is no longer "hard-wired" into the code. For example, to reproduce the "FACTAR total mixing" model one coolant flow channel is defined which is in contact with all sheath and pressure tube sectors. The user can also specify whether mixing between distinct coolant flow channels occurs at the bundle endplates. Since adjacent bundles can be in any geometrical state, this specification must be made for each state pair. For example, the user may choose to represent the nominal bundle state using one coolant flow channel ("FACTAR total mixing"). For the ballooned state (one in which the pressure tube has ballooned into contact with the calandria tube), the coolant between the outer fuel pitch circle and the pressure tube could be considered as distinct from the coolant in the inner flow zone. For the ballooned state with multiple flow channels, the user can specify whether the coolant in the two channels is fully mixing at the endplate before flowing into the next downstream bundle, or it can be specified that no communication exists between each flow channel. This ability has been incorporated to mimic the mixing options in the CHAN[14] code.

The transition from one geometrical state to another (*e.g.*, from a nominal bundle to a ballooned bundle) is coded in a general manner to facilitate future upgrades. Each state is defined with its own representation, and so can model a different arrangement of fuel pins with a different nodalization, a different number of coolant flow channels, *etc.* To accomplish this, the user must define how quantities in each "destination state" are related to quantities from its parent (previous) state. In the example given above, the nominal state consists of one flow channel and the ballooned state consists of two flow

channels. The coolant in the destination (ballooned) state, at the time of the state transition, is specified to initially have the characteristics (*e.g.*, temperature, density) of the coolant in the single flow channel of the nominal configuration. Thereafter, convective energy deposition and mass flow rate variation calculations are performed separately for each coolant channel. In this way, the "FACTAR deformation-based mixing" option[11] from FACTAR 1.x is recreated.

A simulation using FACTAR 2.0 (LOCA) can be performed once all desired geometries have been defined, including view factor matrices applicable for each state, and information related to transforming between states. Two additional input files, one containing initial steady-state conditions *and one* containing transient boundary conditions, are also required. FACTAR will then iterate in order to generate consistent steady-state thermal hydraulic conditions and fuel element temperature profiles. The remaining sequence of calculations, performed at each transient time step, is described in the following sections.

2.3 Dryout and Convective Heat Transfer

Once the thermal hydraulic boundary conditions and local flow direction have been determined, FACTAR begins its channel calculations. First, the dryout status of the current bundle is determined. In previous code versions, the bundle-averaged critical heat flux (CHF) was evaluated from a user-specified correlation, and compared to the actual average heat flux. When the bundle heat flux exceeded the CHF, that bundle and all downstream bundles were assumed to enter dryout. FACTAR 2.0 (LOCA) uses a similar approach; however, due to the ability to model changes in flow direction (as opposed to uni-directional flow), a comparison to the local CHF is performed at every axial location and dryout is not imposed on downstream bundles. All surfaces within the bundle (*i.e.*, all circumferential sheath and pressure tube sectors) are assumed to enter dryout at the same time.

The convective sheath-to-coolant heat transfer coefficient is calculated for each modelled sector from a range of correlations, based on the dryout status, surface temperature, the temperature of the coolant in contact with that sector, the local quality, coolant mass flux and pressure. The correlations and logic of application, similar to those employed in one option of TUF[12], represent an accurate assessment of heat transfer over the entire range of surface/coolant conditions:

Negative heat transfer (heat added to surface from coolant):

- Subcooled liquid — Dittus-Boelter, Kay
- Two-phase — Aniev (condensation)
- Vapour — Hadaller or Aniev, depending on surface temperature

Positive heat transfer:

- Subcooled liquid — Dittus-Boelter, Kay
- Nucleate boiling — Chen
- Transition boiling — McDonough
- Film boiling/convection to vapour — Heineman

The same correlations and logic are used to evaluate the heat transfer coefficient from the pressure tube to the coolant. The local (sector) calculations are again performed for consistency with a future two-dimensional, circumferential temperature solution; since the current version uses a one-dimensional thermal model, the heat transfer coefficients are averaged to provide the single value used in the temperature calculation. The coolant temperature could also, in general, vary around the periphery of each element and/or pressure tube; these values are also averaged in a manner to ensure the correct total convective heat flux leaves each fuel element.

2.4 Fuel Model

Fuel thermal and mechanical characteristics are calculated by a modified version of the fuel performance code ELOCA.Mk4[2,3]. ELOCA is called for each modelled pin in sequence (from innermost to outermost). This component takes as boundary conditions:

- the average convective sheath-to-coolant heat transfer coefficient and average coolant temperature (used to calculate convective heat flux);
- the thermal radiation heat flux (described in more detail in Section 2.5);
- the coolant pressure (used to calculate radial and axial sheath strain);
- the normalized overpower transient (used to scale the volumetric heat generation); and
- oxygen flux (for Zircaloy/steam reaction).

ELOCA models in fine detail sheath deformations arising from thermal, elastic and plastic strains; fuel thermal expansion and cracking; radial variations in fuel and sheath temperature; and sheath failure mechanisms including beryllium-braze assisted crack penetration and athermal strain. The most significant change made to this set of subroutines from FACTAR 1.x relates to data handling. In FACTAR 1.x, element characteristics for a particular pin were stored in data files after each call to ELOCA and retrieved for that pin at the beginning of the next thermal hydraulic time step. In FACTAR 2.0 (LOCA), this data handling is done entirely in memory using customized data structures. This significantly reduces CPU time (by a factor of five approximately), and can reduce real run time even more in a distributed computing network where a central file server is used to perform all I/O operations.

The exothermic Zircaloy/steam reaction at the sheath outer surface is evaluated during the iterative temperature solution in ELOCA. A number of possible options are available, as specified by the user: the Urbanick-Heidrick, Prater-Cathcart and Sawatzky correlations are all available, as is the mechanistic model FROM3[15]. The FROM model solves the moving boundary diffusion equations for oxygen within the Zircaloy sheath, including the formation/deletion of a beta layer. This model automatically accounts for the ability of oxygen to diffuse through the outermost oxide layer, thus limiting the amount of energy released by the reaction.

2.5 Pressure Tube / Calandria Tube Model

After temperatures and deformations for all fuel elements in a particular bundle are calculated, the thermal and mechanical behaviour of the pressure tube and calandria tube are assessed. This model is essentially identical to the one used in the FACTAR 1.x code series (FACTAR 1.2 and later): a finite volume, radial solution of the transient energy conservation equation is used to calculate the thermal response. Pressure tube strain is evaluated through solution of Shewfelt's equations[6] for strain of Zr-2.5wt% Nb pressure tubes. A sub-time step (with respect to the thermal hydraulic time step) is calculated based on numerical stability considerations, and iteration is performed to ensure consistent nodal temperatures and thermal properties. The largest changes made in FACTAR 2.0 (LOCA), with respect to the pressure tube/calandria tube model, have been to generalize the algorithm to allow user-input thermal properties, and to model more than two tubes. These generalizations were added to facilitate validation against the BTF[16] series of experiments which use a four layer thermal shroud instead of a prototypic CANDU pressure tube/calandria tube geometry.

2.6 Thermal Radiation

The calculation of thermal radiation between surfaces in FACTAR 2.0 (LOCA) is significantly different than in previous versions of the code. FACTAR 1.x applies a concentric cylinder model wherein radiation is considered only between adjacent rings of elements or between the pressure tube and the outer ring. Radiation between pins within a ring is not accounted for as all pins within a ring are assumed to have the same temperature profile. This approach is most appropriate for axisymetric geometries with axisymetric boundary conditions where temperature variations between pins in a ring do not exist as is the case for

FACTAR 1.x analysis. A more general approach is required to accurately predict radiation heat transfer for conditions which depart from this (*e.g.*, slumped bundle or sagged pressure tube geometries).

In FACTAR 2.0 (LOCA) radiative heat transfer between each surface (defined by a circumferential sector on fuel elements), or surrounding tubes with all other surfaces in the cross section, is determined. Axial radiation is not considered. A view factor matrix is input to FACTAR for each geometry or state under consideration in the analysis. This matrix defines the fraction of energy leaving each surface which is incident upon all other surfaces based on the assumption of diffuse radiation. A stand alone utility code, VIEWFACT, has been created to generate the required view factor matrices. The utility can accept any arrangement of circular pins distributed within a circular tube. Within FACTAR, the view factor matrix for each state is combined with the surface emissivities supplied through the geometric input deck and the associated radiation matrix is determined. The radiation matrices are inverted before the transient calculations are initiated. At each time step, the net radiative heat flux for each surface is calculated from the inverted radiation matrix, the surface emissivities and the surface temperatures. The heat fluxes are applied as boundary conditions for the fuel (ELOCA) and pressure tube/calandria tube thermal models. This treatment is similar to that used in detailed bundle codes such as HOTSPOT[4] and SMARTT[5].

2.7 Hydraulic Calculations

Up to this point in the calculational sequence, the thermal response of channel components has been calculated using hydraulic conditions evaluated at the previous time step. The thermal hydraulic calculations are all performed using the most recently calculated component temperatures. The sequence of thermal hydraulic calculations is described below.

2.7.1 Flow Distribution

Due to sheath and pressure tube strain, the area available for coolant flow changes with time. The change in component area in contact with each modelled flow channel over the last time step is evaluated, and the flow area is updated (*i.e.*, the area of flow channels in contact with the pressure tube is increased due to pressure tube strain, while the area of flow channels in contact with fuel elements decreases as a result of sheath strain).

The fraction of the total exit flow from the upstream bundle that enters each downstream flow channel is proportional to the relative downstream flow area, and to the square root of the inlet coolant density. These dependencies arise from the Bernoulli equation assuming equal pressure drop in each flow channel. The model for this flow distribution is unchanged from FACTAR 1.x.

2.7.2 Inlet Enthalpy

The inlet enthalpy to the current bundle is assessed based on the exit enthalpy from the upstream bundle (or the applied inlet enthalpy boundary condition in the case of the first bundle calculation), and on the user specified flow channel mixing options. As discussed in Section 2.2, for each state pair it must be specified how the flow channels communicate with each other. For a given state pair, the upstream coolant channels which contribute to the inlet enthalpy for each downstream channel are specified. For example, if the coolant flows from a ballooned bundle modelled with four flow channels to a nominal bundle modelled with two flow channels, it could be specified that all four channels mix at the endplate and both of the downstream channels experience the same average inlet enthalpy; alternately, two specific upstream channels may mix together to contribute to the inlet enthalpy for one downstream channel, and the other two channels mix to produce an average inlet enthalpy for the other downstream channel. The logic is also general enough to support partial mixing of coolant channel enthalpy, so that a specified fraction of the coolant flow in one upstream channel is diverted to the inlet of a particular downstream channel.

2.7.3 Coolant Energy Equation

Once the inlet flow with associated enthalpy to a particular flow channel has been calculated, the change in enthalpy along the axial segment is calculated by solution of the discretized transient coolant energy equation. The convective heat transfer at solid surfaces is evaluated by integrating the instantaneous surface heat fluxes calculated by ELOCA and the pressure tube model over their sub-time steps.

2.7.4 Coolant Flow Rate

The change in coolant flow rate along the channel at a given time is calculated by solution of the transient mass conservation equation for a homogeneous mixture. The change in coolant density arising from temperature variations and phase changes is included. The change in coolant flow rate along the channel is significant during periods of rapid phase change (such as during the blowdown period of a large break LOCA), but is relatively small for single-phase vapour cooling (although it is always calculated). This model is new to FACTAR 2.0 (LOCA); FACTAR 1.x assumed that the coolant flow rate was axially invariant at a given time step, although it did vary with time. The flow boundary condition for FACTAR 1.x was calculated as the average flow rate predicted by TUF at each time step, so that rapid changes in coolant flow rate with time were captured, but not to the level of detail possible in FACTAR 2.0 (LOCA).

The solution of the coolant mass and energy equations completes the thermal hydraulic portion of the channel calculation. The code moves on to the next downstream bundle, and repeats the calculations described in this section. After calculation at the last bundle in the channel, the time variable is incremented and the code marches through time until the end of the simulation.

3. OTHER CODE IMPROVEMENTS

A number of other improvements have been made in FACTAR 2.0 (LOCA) not pertaining to the physical modelling. The generalization of the code to represent more general geometries (the separation of data from physics) has been discussed. All input files (with the exception of the steady-state file) are in free format (position of data is irrelevent), and support the inclusion of comments at arbitrary locations for the convenience of analysts. Other improvements are related to software engineering changes:

- increased modularity: the number of functions and subroutines has been increased by approximately 50%, to improve code maintainability. The average length of a subroutine has been decreased to facilitate understandability, and the logic has been restructured such that each subroutine performs a single, well-defined calculation.

- tighter data control: the FORTRAN statement `IMPLICIT NONE` has been added to every source module, which requires that all variables used have an explicit declaration. These declarations have been placed in standard headers at the top of each routine that also describe the purpose of the routine and its place in the calling sequence. Each declaration line specifies the variable type and also includes a description of the purpose of the variable as an in-line comment. These headers greatly simplify the task of a programmer unfamiliar with FACTAR who is trying to understand the functioning of the code; this situation commonly arises due to the requirement to have source code changes verified by an individual who did not originally perform the work. Common block definitions, particularly those relating to the generalized geometry, have largely been placed in INCLUDE files to eliminate the possibility of common block mismatches.

- language changes: certain FORTRAN-90 features have been added to the code, where appropriate, to simplify its understandabilty. Examples of this include whole array operations (such as initialization), some extremely useful intrinsic functions used for CHARACTER data manipulation (`TRIM`, `LEN_TRIM`, *etc.*), use of user-defined structures to hold large amounts of related data (such as that used to collect fuel element data and save it to memory rather

than to file), and use of the "double colon" declaration which can be used to specify *all* variable attributes in a single line, preventing later confusion (for example, the syntax `INTEGER, PARAMETER :: C_to_K = 273.15` to declare a temperature conversion factor).

- coding style: elimination of most GOTO statements and line labels (except for FORMAT statements) to promote structured coding; use of longer and more meaningful (*i.e.*, self descriptive) variable and subroutine names.

FACTAR 2.0 (LOCA) also performs many more self-consistency checks than did its predecessor. Post-processed mass and energy balances are performed for all specified bundles, and any imbalances are reported to the user. The level of these balances ranges from nodal energy balances for the fuel and pressure tube thermal solutions, to global bundle energy balances. Correct transfer of data from one module to another is also ensured through these checks. More calculated data is reported to the user, allowing the analyst to more fully understand the results of the simulation. The user has also been given more control over the data printed to the output file, which can be used to tailor the output for a specific type of study. The ability to vary fuel thermal properties for sensitivity studies has been added; additional detailed information can also be generated for input to formal uncertainty analysis methods, such as the Discrete Adjoint Sensitivity Method[17].

The coding changes described above have the effect of making the code easier to maintain, thus reducing the largest cost in any code lifecycle. They also instill greater confidence that the code is performing properly, and allow a more thorough analysis of fuel channel behaviour under postulated accident conditions. The changes have the added benefit of making the code easier to verify and validate, and in this case also improve code performance.

4. APPLICABILITY, VERIFICATION AND VALIDATION

FACTAR 2.0 (LOCA) has been designed and tested for large break LOCA scenarios in CANDU reactors. It is also capable of modelling any less severe transient which avoids significant periods of flow stratification, such as transition break LOCAs. The current code version does not include several high-temperature (*i.e.*, post fuel or sheath melting) models which would be necessary to represent more severe cases, such as a large break LOCA with coincident loss of emergency coolant injection. However, the design of this code has considered the need to implement certain models in the future, such as Zircaloy/UO_2 interaction, bundle slumping and fuel oxidation[18]. Coding has been performed such that addition of these models can be done in a modular fashion with minimal impact on the existing code. It is intended to extend the code's applicability to these scenarios by 1997, in the code version "FACTAR 2.0 (LOECI)".

Testing and development verification were performed at all stages of code development to ensure that each change was correctly made. Comparison of code results with analytical solutions, hand checks and cross-code comparisons with validated simulation codes has been performed to demonstrate that FACTAR 2.0 (LOCA) functions properly. Formal validation, following the Canadian nuclear industry standard Validation Matrix approach[19], is currently underway and will be reported in the near future.

5. SUMMARY

This paper has discussed the fuel and channel thermal/mechanical response code FACTAR 2.0 (LOCA), which is the successor to the FACTAR 1.x code family. Significant improvements to the code, ranging from constituent models to code architecture, have been described. An overview of the calculational sequence used in FACTAR 2.0 (LOCA) has been given, along with the range of applicability of the code.

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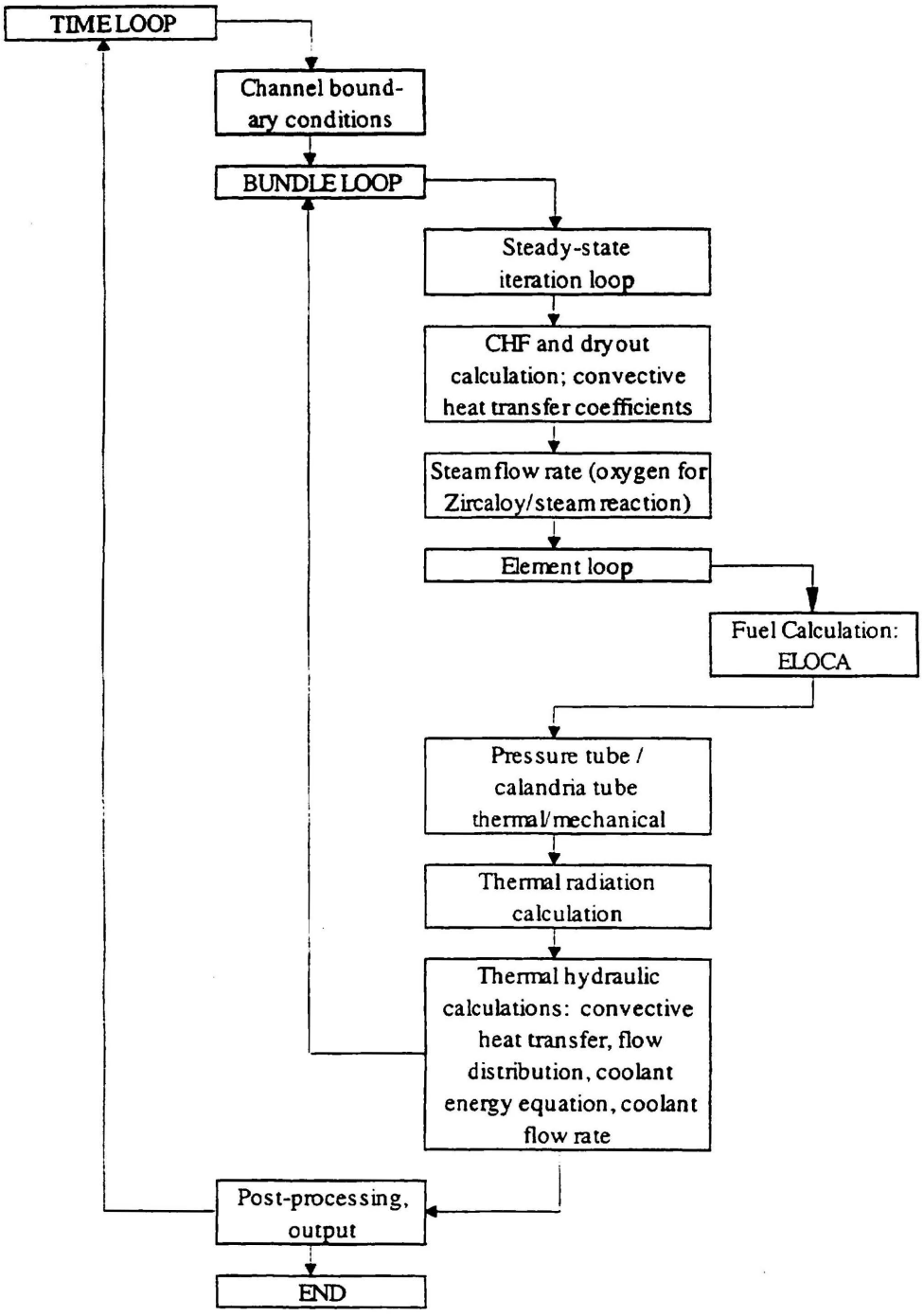

Figure 1: Overview of calculational sequence in FACTAR 2.0 (LOCA)

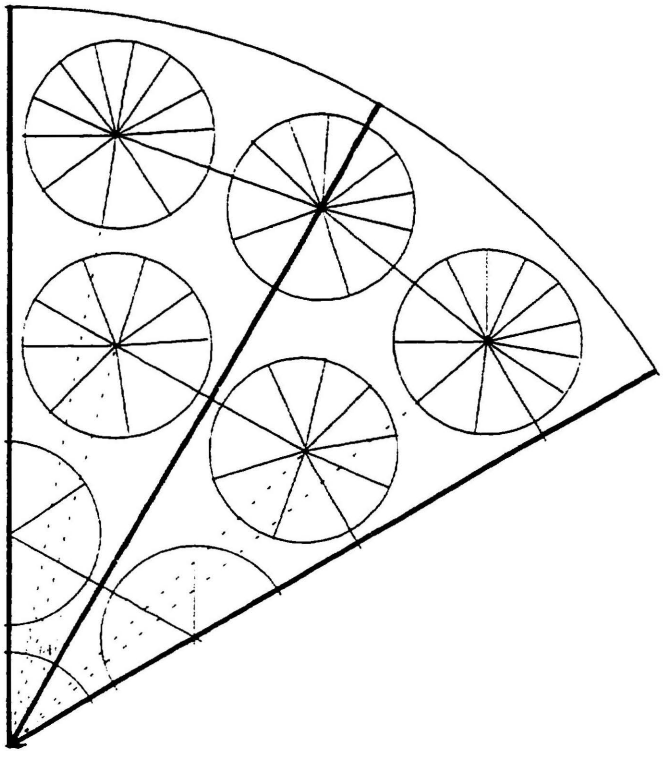

Figure 2: Sample Geometrical Representation used in FACTAR 2.0 (LOCA) for a 37-element Bundle (two 1/12th symmetric wedges)