# The Eloca Fuel Modelling Code: Past, Present And Future

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## ABSTRACT

ELOCA is the Industry Standard Toolset (IST) computer code for modelling CANDU fuel under the transient coolant conditions typical of an accident scenario. Since its original inception in the early 1970's, the code has undergone continual development and improvement. The code now embodies much of the knowledge and experience of fuel behaviour gained by the Canadian nuclear industry over this period. ELOCA has proven to be a valuable tool for the safety analyst, and continues to be used extensively to support the licensing cases of CANDU reactors. This paper provides a brief and much simplified view of this development history, its current status, and plans for future development.

## 1. INTRODUCTION

ELOCA is an acronym for "Element Loss Of Coolant Analysis". Simply put, ELOCA is a Fortran code that calculates the temperature of a single CANDU fuel element and the likelihood of fuel sheath failure under the adverse cooling conditions of an accident. This information is fed to other "downstream" computer codes such as SOURCE, SOPHAEROS and SMART, to calculate the fission product source term, the release of fission products to the heat transport system, to containment and ultimately, the radiological dose to the public.

### 1.1 Modelling CANDU Fuel

Modelling CANDU fuel under Normal Operating Conditions (NOC) is done using ELOCA's sister code, ELESTRES [1] (which is also an IST code). Despite its many capabilities, ELESTRES is fundamentally a steady-state code and does not model the rapidly changing conditions that the fuel experiences during a postulated loss of coolant accident. In a typical analysis, ELESTRES models the fuel element from the beginning of its irradiation in the reactor to the start of the accident transient. ELESTRES then passes data on the physical condition of the fuel, at the start of the transient, to ELOCA.

These data provide the initial conditions required for the ELOCA simulation of the accident transient.

The physical components modeled by ELOCA are the fuel pellets and fuel sheath. ELOCA models the heat generation inside the fuel pin and the transport of heat (by diffusion) through the fuel to the fuel-to-sheath boundary, across the fuel-to-sheath boundary, through the sheath, and into the coolant. The time dependant boundary conditions are: the coolant temperature, the sheath-to-coolant heat transfer coefficient, the coolant pressure, and the linear power of the fuel element. These boundary conditions are usually supplied via separate thermalhydraulic and physics calculations (or via direct measurements).

The heart of the problem of modelling CANDU fuel is the strong feedback between the temperature of the fuel and the mechanical interaction between the fuel and the sheath. The circle of interactions is as follows:

- The temperature of the fuel is a function of the fuel-to-sheath heat transfer coefficient,
- which is a function of the fuel-to-sheath interface pressure or (fuel-to-sheath gap),
- which is a function of differential thermal expansion between the fuel and the sheath, and of the internal gas pressure,
- which in turn is a function of the fuel and sheath temperature.

Thus, any adequate model of CANDU fuel behaviour must not only include a good thermal model for the heat transport within the fuel and sheath, but must also contain a model of the mechanical behaviour of the Zircaloy sheath. The mechanical behaviour of the sheath determines the fuel-to-sheath interface pressure (or gap size), and hence the fuel-to-sheath heat transfer coefficient.

The situation is further complicated by the straining and creep of the sheath under the mechanical loads imposed by the fuel, the coolant, and internal fission gas, and the potential for the sheath to lift away from the fuel under accident conditions.

An additional feedback mechanism arises from the potential diffusion of fission gas out of the fuel matrix into the internal voidage of the fuel element, reducing the fuel-to-sheath interface pressure, and the thermal conductivity of the gas in the gap. The diffusion mechanism is also strongly dependant on the fuel temperature.

Further refinements include: the ability to calculate the Zircaloy/steam interaction and account for the extra heat of oxidation, and the ability to predict the timing of sheath failure.

## 2. EVOLUTION OF THE ELOCA CODE

This paper describes the functionality of the ELOCA code via its development history. In what follows the major code releases are identified along with the major developments that distinguish the code versions. A brief description is provided of each model or feature as it was added to the ELOCA code along with the rationale for its inclusion. The restrictions of space require that these descriptions be brief, but it is hoped that this paper will give the reader both an impression of the depth of work put into the ELOCA code over the past 30 years, and a general understanding of the code's current capabilities.

## 2.1 ELOCA.Mk1(1) 1975 (2)

Work began to create a computer code to model the transient behaviour of CANDU fuel at AECL's Chalk River Laboratories in the early to mid 1970's. Sills wrote the first documented version of the ELOCA code in 1975. The model was essentially one-dimensional and treated the fuel element as an infinitely long cylinder of fuel with a concentric Zircaloy sheath. This initial version of the code included models for:

Heat generation and diffusion

The calculation of the heat generation rate as a function of position within the fuel and burnup usually requires the use of several reactor physics codes. For the ELOCA code, however, the assumption is made that the normalized radial profile of the heat generation rate remains unchanged for the short duration of the transient. Information on this radial profile was passed to the ELOCA code from the NOC fuel modelling code ELESIM(3). ELESIM calculated this radial profile using lookup tables based on a previously conducted physics calculations. The radial profile was then scaled by the ELOCA code to give the correct linear rating of the fuel element, as specified in the input file.

The radial heat diffusion through the fuel and into the coolant was calculated using a semi-implicit (Crank-Nicholson type) finite-difference solution method. The nodalization consisted of nodes placed on the boundaries of concentric radial annuli. One hundred annuli were used within the fuel pellets. Outside the fuel pellets there was: a single annulus for the fuel-to-sheath gap, a single annulus for the sheath, and an additional node located in the coolant for the specification of the coolant boundary condition.

*Fuel-to-sheath heat transfer*

The transfer of heat from the fuel to the sheath was modelled using the correlation of Ross and Stoute [2]. This model treated the heat transfer between the fuel and the sheath as three separate components:

(1) At this time "Mk1" was not part of the name of the code.
(2) The dates given here are approximate for when the code versions were in general use.
(3) ELESIM was a precursor of the ELESTRES code [1].

- solid-to-solid conductance between the fuel and sheath, which is a function of the surface roughness of the fuel and sheath, and of the fuel-to-sheath interface pressure,
- gas conductance across the fuel-to-sheath gap, which is a function of the surface roughness, gap gas composition, and gap gas temperature, and
- radiative conductance, which is a form of Stefan's law and is a function of the fuel and sheath temperatures.

*Thermal expansion of the fuel (including cracking)*

The first version of ELOCA used a correlation by Burdick and Parker [3] to calculate the thermal expansion of the fuel.

For the purposes of the thermal expansion model, the assumption was made that the fuel was an incompressible solid with zero tensile strength. The volume of fuel in each annulus and the volume of an annulus were tracked separately and the difference between these volumes was interpreted as the voidage caused by fuel cracking. The change in volume of fuel within an annulus due to thermal expansion was easily calculated from the correlation. The change in volume of the annulus was more difficult to calculate, as the annuli must remain contiguous. This problem was addressed by calculating the expansion of each annulus width, and then redistributing the position of each annulus from the centre of the fuel outwards. If necessary a void was formed at the centre of the fuel in order to ensure continuity of the annuli.

*Internal Gas Pressure*

The amount of gas inside the fuel sheath was provided to ELOCA as input from the NOC computer code ELETRES. The gas pressure within the sheath was calculated as a function of the volume of the internal element voidage and temperature using the ideal gas law. For this version of ELOCA the assumption was made that there was no additional fission gas release from the fuel to the voidage during the short period of the transient.

*Sheath Model*

The sheath model in this first version of ELOCA was a relatively simple one-dimensional model, in which the strain is assumed to be uniform along the length of the fuel element. In comparison to the sheath, the ceramic fuel was regarded as incompressible and, as it expanded thermally, it imposed a strain upon the sheath. The corresponding stress in the sheath was calculated from the constitutive equations for a thin-walled cylinder of the appropriate material properties. The sheath underwent elastic deformation until the yield stress was reached, after which it underwent permanent plastic strain. Additional plastic strain due to creep of the sheath was determined from creep rate correlations derived from experimental data reported by Hardy [4].

*Sheath Oxidation*

The thickness of the oxide formed on the outside of the fuel sheath was calculated using a parabolic growth rate with coefficients from unpublished work by Urbanic. The heat of oxidation was included as an additional heat generation factor applied to the outside node of the fuel sheath. The reduction in fuel sheath thickness due to oxidation was also included in the sheath strain calculation.

*Oxide Strengthening*

The diffusion of oxygen in the Zircaloy sheath has the effect of strengthening the sheath and hence, reducing the creep rate. The reduction in the creep rate was accounted for using empirical relations derived by Hobson and Rittenhouse [5].

## 2.3 ELOCA Mk2, 1978

The most significant advancements incorporated into the ELOCA.Mk2 code [6] were the Sills and Holt micro-structural sheath creep model [7] and the addition of the Køhn and Clendening model for beryllium-assisted crack penetration of the sheath [6]. In addition, the fuel thermal expansion correlation was updated to that provided by the MATPRO 9 handbook [8], and the sheath oxidation model was also updated to use the parabolic correlations proposed by Urbanic and Heidrick [9].

*Microstructural Sheath Deformation Model*

The calculation of the fuel-to-sheath heat transfer coefficient requires an accurate model for the deformation behaviour of the Zircaloy sheath. Sills and Holt [7] developed the microstructural sheath creep model to meet this requirement. The model was initially developed separately from ELOCA as the NIRVANA code [10], and was independently tested against a large number of sheath strain experiments. The model included components for: high temperature annealing (recrystallization), changes in the alpha-phase fraction, and changes in grain size. The high-temperature creep behaviour of the sheath was modelled as three separate components: dislocation creep, grain- or phase-boundary sliding, and strain due to phase transformation. The assumption was made that the $ZrO_2$ formed on the outside of the sheath did not carry any tensile load, and the thickness of the load carrying portion of the sheath was adjusted to account for oxidation. At this stage the model did not include the effects of diffused oxygen on the sheath material properties (i.e. oxide strengthening).

*Beryllium-Assisted Crack Penetration Model*

A generic feature of the CANDU fuel design is that appendages such as bearing pads and spacers are attached to the sheath by beryllium brazing. Under normal operating conditions, this method of attachment has proved to be both reliable and robust. Under high temperature and stresses, the presence of beryllium has been shown to accelerate the propagation of cracks in the sheath leading to sheath failure. This phenomenon was investigated in an experimental program conducted by Køhn and Clendening [6] while working at Westinghouse Canada. They developed a stochastic model for the propagation rate of sheath cracks in the presence of beryllium, as a function of stress and temperature. Coupling this model with the ELOCA code allowed for the prediction of the probability of sheath failure by this mechanism.

## 2.4 ELOCA A 1978

At less than 0.5 m, the length of a CANDU fuel element is relatively short in comparison to other fuel types; hence in many situations axial variations (in ELOCA boundary conditions) along the length of the fuel element are small and a one-dimensional model is adequate. Under some accident scenarios, however, the fuel element may experience large axial variations in the coolant conditions and, for elements near the ends of the fuel channel, the axial variation in neutron flux may also be significant.

To account for axial variations in coolant temperature and linear power, Tayal et al. [11] modified a development version of ELOCA.Mk2 to include axial segmentation. In this implementation the user was able to divide the fuel into a number of axial segments and specify different linear power, coolant conditions, and sheath material properties for each segment.

ELOCA A underwent parallel development, and was successfully used by safety analysts at AECL until the late 1980's, when the decision was made to merge the capabilities of the ELOCA A code with the new ELOCA.Mk4 code version.

## 2.5 ELOCA.Mk3 1983

The most significant model development for ELOCA.Mk3 was the extension by Walsworth, Sills, and Sagat, of the sheath microstructural creep model (NIRVANA) to include the effects of oxidation and oxide strengthening [12]. This model, known as TOSS (Transient Oxidation Strain Simulation), simulated the sheath as three layers: $ZrO_2$, oxygen stabilized $\alpha$-Zr, and the substrate (either $\alpha$ or $\beta$ phase Zircaloy depending on the temperature). The model included a component to account for cracking of the oxide layer.

## 2.6 ELOCA.Mk4 1984

Developments for ELOCA.Mk4 saw a greater emphasis on prediction of sheath failure, and included the addition of a number of fuel sheath failure mechanisms [13]. In total, ELOCA.Mk4 included six criteria used for the prediction of sheath failure:

- Sheath overstrain: the sheath was deemed to have failed if the sheath strain exceeded a user defined limit (default value of 15%),
- Localized overstrain at oxide cracks: the sheath was deemed to have failed if the strain under an oxide crack exceeded the overstrain limit,
- Excessive sheath creep rates: the sheath was deemed to have failed if the sheath creep rate exceeded $10^{-1}s^{-1}$,
- Low Ductility Sheath Failure: the sheath was deemed to have failed if the strain exceeded 0.4% when the volume fraction of uncrystallized $\alpha$-Zr still exceeded 5%. The zircalloy crystallization process was modelled as part of the NIRVANA code [10],
- Beryllium assisted crack penetration: the sheath was deemed to have failed when the calculated probability of failure exceeded 0.95, and
- High fuel enthalpy: the sheath was deemed to have failed, because of fragmentation of the fuel, if the average radial energy deposited in the fuel during a power pulse exceeded 838 kJ/kg $UO_2$ (this failure criterion is no longer used).

Other modifications for ELOCA.Mk4 included:

- Further extension of the sheath creep model to include alpha-beta transformation kinetics,
- Extension of the creep model to include the effects of oxidation over the entire temperature range,
- Modification of the beryllium-assisted crack penetration model to include the effects of oxidation,
- Modifications to the thermal solution to improve computer run time.

## 2.7 ELOCA.Mk4S 1988-1990

With ELOCA.Mk4S, de Vaal, Walsworth, and Carlucci merged the capabilities of ELOCA A with ELOCA.Mk4 to produce a code that allowed the fuel element to be divided into twenty axial segments, to account for both axially varying boundary conditions and sheath material properties (for example, braze heat affected zones). To maintain the same functionality as ELOCA A, the number of available sheath oxidation models was increased to include the parabolic growth correlations of Urbanic & Heidrick [9], Baker & Just [14], and Sawatzky & Prater [15].

## 2.8 ELOCA.Mk5 1992

The presence of fission gas in the internal voidage of the fuel element was known to increase the temperature of the fuel as it reduced the fuel-to-sheath heat transfer coefficient. The diffusion of gas out of the fuel matrix is a slow process for many accident scenarios, so it was reasonable to assume there was insufficient time during the transient for additional release of gas to the fuel-to-sheath gap. However, the diffusion of fission gas within the fuel matrix is strongly dependent on the fuel temperature and, in some instances, the additional release of fission gas during the transient may be sufficient to influence the fuel behaviour.

In the late 1980's, MacDonald et al. [16] developed the FREEDOM code to model fission gas production and diffusion to the fuel-to-sheath gap during a transient. The FREEDOM model included models for the following phenomena:

- Fission product formation,
- $UO_2$ grain growth (both equiaxed and columnar),
- The collection of fission gas by moving grain boundaries (grain boundary sweeping),
- Fission product diffusion (the Booth model),
- Fission product release by bubble growth and grain face separation, and
- Fuel swelling due to fission gas bubbles.

The FREEDOM model was linked to the ELOCA code and released as ELOCA.Mk5 by Walker [17].

Initially, the coupling to FREEDOM could only be implemented for simulations using a single axial segment (i.e. 1-D). Later, de Vaal extended the coupling to allow modelling of up to twenty axial segments and released the code as ELOCA.Mk5S.

Other developments for the ELOCA.Mk5 release included the addition of Sawatzky's [18] criterion for sheath failure due to oxygen embrittlement, and coupling to the first version of the sheath oxidation model FROM (Full Range Oxidation Model) via a VAX/VMS network link (more information on FROM is provided below).

## 2.9 ELOCA.Mk6 1994

Up until ELOCA.Mk6 [19], the time of the fuel sheath failure had marked the end point of an ELOCA simulation. With inclusion of the Lian et al. [20] post-sheath-failure model, it became possible to simulate the behaviour of the fuel element during the period of post failure depressurisation and beyond. The post-sheath-failure model included components for:

- Depressurization of the fuel element,
- Convective-diffusion model for post-failure transport of fission products to the coolant, and

- Changes in the fuel-to-sheath gap conductance.

In addition to the post-sheath-failure model, ELOCA.Mk6 also included a “pellet bottoming” model, by Arimescu [19]. This model corrects for the non-uniform fuel-to-sheath heat transfer resulting from the fuel pellets dropping off centre in a horizontal fuel sheath.

## 3. THE IST INITIATIVE

In the late 1990’s, there was an industry-wide initiative to adopt a unified approach to qualify the computer codes used in safety analysis. Up until this time, the development of safety analysis codes had been conducted independently by several organisations and groups; consequently, there was a profusion of codes in use. Several codes fulfilled the same or similar tasks and it was realised that the cost of qualification could be substantially reduced by choosing a standard set of codes for use in safety analysis. A steering committee consisting of representatives from the Canadian nuclear utilities and AECL was formed to select the necessary codes, and coordinate qualification and future code development. This set of codes was termed the Industry Standard Toolset (IST).

The ELOCA code was chosen as the IST tool for the analysis of CANDU fuel under accident conditions. Under the coordination of the IST steering committee, a list of requirements for an IST version of ELOCA was formulated and a cycle of staged development was initiated, culminating in a series of validation exercises completed in 2001.

### 3.1 ELOCA-IST 1.0 1998

The starting point for the new IST code was ELOCA.Mk6. In the first stage of development, ELOCA was fully coupled to the sheath oxidation model FROM_SFD (Full Range Sheath Oxidation Model _ Severe Fuel Damage).

FROM_SFD was developed from the second version of FROM, FROM2 [21], in the early 1990’s by Conlon et al. The FROM model differs from the other parabolic growth rate models available in ELOCA as it is a mechanistic model for the diffusion of oxygen into the Zircaloy sheathing. FROM_SFD is not only capable of modelling the Zircaloy oxidation on the outside of the sheath, it is also capable of simulating the Zircaloy/$UO_2$ interaction on the inside of the sheath.

The model divides the fuel sheath into a number of distinct regions, depending on the oxidation state and the interaction with the fuel. A moving boundary finite element scheme is used to solve the oxygen diffusion equations in each region and calculate the oxygen concentration as a function of position within the sheath. In the initial implementation within ELOCA, only the information on the outside sheath oxidation was used by ELOCA. The information on the $UO_2$-Zircaloy interaction was calculated by FROM_SFD, but was not passed to ELOCA or used.

ELOCA-IST 1.0 also included an extension by Arimescu to the existing sheath creep model, to extend the applicability of the Zircaloy creep model to temperatures as low as 600 K.

### 3.2 ELOCA-IST 1.1 1998

The next major step in the ELOCA-IST development was the implementation of a two-dimensional temperature solver. The generalized 2-D temperature solver, called TEMDRIV, was developed independently of the ELOCA code by Carlucci and Gauld in the early 1990's, and uses a finite control volume method to solve the heat transport equations within the fuel and sheath. This 2-D temperature solver allows for circumferential temperature gradients to be applied to the outside of the fuel sheath, i.e. it allows for simulations in which the top of the fuel sheath is hotter than the bottom.

It should be noted that the sheath strain calculation remains fundamentally 1-D and is based on an area-averaged sheath temperature. Also, the older 1-D temperature solver was retained as an option within the code to ensure backwards compatibility with previously generated input files.

### 3.3 ELOCA-IST 2.0 1999

The next development stage did not include any changes to the ELOCA functionality, but did include major changes to the internal structure of the code.

The boundary conditions for ELOCA are usually provided by other codes such as the thermalhydraulics code, CATHENA. In fact, there is strong feedback between the phenomena modelled by ELOCA and the thermalhydraulics of the fuel channel. To fully capture this feedback, it was desirable to be able to link ELOCA directly to these codes via a simple subroutine call, and to exchange information between the codes at arbitrary time intervals. An additional requirement was that it should be possible to run several ELOCA models simultaneously to simulate part, or a whole, fuel channel (or even a whole reactor core).

The existing ELOCA program structure did not lend itself to being easily used in this fashion. Also, the extensive use of COMMON block data structures meant that the code could not be easily modified to run several separate ELOCA models, as each separate model would attempt to access and modify the same data stored in the COMMON blocks. To overcome these problems, the COMMON block data structures were removed and the ELOCA source code was broken up into several subroutines that can be easily called from another code. When using ELOCA alone, a driver program, supplied as part of the standard ELOCA configuration, controls the subroutines.

### 3.4 ELOCA-IST 2.1 2001

It had been decided, as part of the IST initiative, that the preferred tool for the calculation of fission product formation and release would be the new code SOURCE IST [22]. Consequently, the FREEDOM fission gas release model was removed from ELOCA, on the understanding that ELOCA-IST and SOURCE IST would be coupled together at a future date.

In addition, the fuel thermal expansion model was changed to that provided in the MATPRO 11 handbook [23] to be consistent with the ELESTRES-IST code.

The final modification for ELOCA-IST 2.1 was to package the data passed between the main ELOCA subroutines into Fortran 90 data structures. Packaging the data into structures in this way, and placing the structures into “modules”, greatly simplified the calls to the ELOCA subroutines, making the code easier to maintain and helping ensure data integrity.

### 3.5 The verification and validation of ELOCA-IST 2.1

As part of its qualification, ELOCA-IST 2.1 underwent an extensive line-by-line verification. While the verifiers identified a large number of issues, mainly concerned with legacy coding practises and difficulties with the internal code documentation. None of the issues raised were regarded as serious enough to warrant immediate correction and ELOCA-IST 2.1 was deemed ready for validation. The verification findings were documented and used as the basis for the next stage in the ELOCA development.

To date, ELOCA-IST 2.1 has been validated against three separate effects datasets for the phenomenon of sheath oxidation (including nearly 500 individual oxidation experiments), five separate effects datasets for the phenomenon of sheath failure (including 187 individual sheath ballooning experiments), and 12 fully integrated in-reactor experiments. In addition, the code has been validated against four power pulse experiments conducted in the IGR facility in Russia. The code performed well and no major deficiencies were identified in these validation exercises.

## 4 CURRENT STATUS

Since 2001, ELOCA-IST 2.1 has undergone several incremental upgrades to add greater detail to the output file, include the capability to model dysprosium-doped fuel, and to correct a coding error in the nodalization of the fuel-to-sheath gap. The latest version of ELOCA is ELOCA 2.1c, which was released for use in 2004 December.

## 5. FUTURE DEVELOPMENTS

The next planned version of ELOCA is ELOCA 2.2, which is currently undergoing testing and is scheduled for release in 2005. ELOCA 2.2 will include

- Changes to address the verification findings from the qualification of ELOCA-IST 2.1, and
- Implementation of dynamic memory allocation and further implementation of several new Fortran 95 features, to aid with code maintainability and help coupling with other codes.

The next major step in the ELOCA development cycle will be the coupling of ELOCA with the fission product generation and release code SOURCE IST. Because of the complexity of the two codes, this is a major undertaking and is currently estimated to take two years of development time. It is expected that the version of ELOCA coupled to SOURCE will be released for use as ELOCA 3.0 in 2008.

## 6. CONCLUSIONS

ELOCA is the Industry Standard Toolset (IST) computer code for modelling CANDU fuel under the transient coolant conditions typical of an accident scenario. Since its original inception in the early 1970's, the code has undergone continual development and improvement. This paper provides a brief and much simplified view of this development history, as both a guide to the current capabilities of the code, and to provide some of the rationale for some of the code design decisions taken.

The ELOCA code continues to be an important safety analysis tool and is expected to continue in this role for the foreseeable future. Future development of ELOCA will continue with: improvements to the existing models, extension of its capabilities to model new fuel designs, and continual upgrades of its existing source code to comply with modern programming practices and to improve maintainability.

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