RESEARCH REPORT

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Initial implementation of cladding ballooning model in FINIX fuel performance code

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Summary

In this work, publicly available cladding ballooning model BALON2 was implemented in VTT's in-house fuel performance code FINIX, to enable more realistic simulation of loss-of-coolant accident (LOCA) and other accident conditions in which anisotropic large cladding deformations can be expected to happen. BALON2 is the default ballooning model in widely used transient fuel performance code FRAPTRAN-2.0 by the U.S. Nuclear Regulatory Commission.

Once the model was implemented, a brief initial validation was provided by simulating Halden IFA-650 LOCA experiments 5, 6 and 7 with FINIX and FRAPTRAN-2.0, comparing the results against experimental data. The currently implemented model was able to predict escalation of ballooning similarly to FRAPTRAN-2.0 and provided a conservative estimate of rod bursting against experimental data in two out of three cases. The initiation of ballooning differed significantly between FINIX and FRAPTRAN-2.0, partly due to slight differences in the threshold conditions, as well as due to differences in how the codes calculate standard mechanical deformation prior to ballooning.

FINIX does not yet provide estimates for residual cladding hoop strain, for which both experimental and reference calculation values exist for the purposes of code validation. This is related to fact that the coupling between the ballooning mechanics and standard mechanical solver are still missing. Furthermore, BALON2 model alone does not include all the tools for comprehensive modelling of effects of ballooning, such as models related to flow-area reduction.

This work succeeds in implementing the essential baseline model of cladding ballooning and enables the prediction of rod deformation and failure in LOCA conditions. Future work should be aimed towards finalizing the linkage between the BALON2 model data structures and the rest of FINIX, in order to provide estimates of residual hoop strain for further validation. Additional validation cases are available as well, and some parts of the code (such as burst stress criterion) could be revisited to further assess differences between FINIX and FRAPTRAN-2.0. The newly implemented LOCA model should improve the LOCA prediction capabilities of FINIX in coupled applications as well, although a thorough validation of FINIX transient modelling is advised prior to that.

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Contents

1. Background

In light water reactors (LWRs), a nuclear fuel rod comprises pellets encased in cladding. These pellets, typically made of uranium dioxide (UO2), undergo nuclear fission to produce heat energy. The cladding serves the crucial role of containing radioactive materials and facilitating the transfer of heat generated by the pellets to the surrounding coolant. Zirconium based alloys are commonly chosen for cladding due to their robust corrosion resistance, sufficient strength, and low neutron absorption rate.

During the design phase of nuclear reactors, ensuring the structural integrity of the cladding under accident conditions, such as Loss of Coolant Accidents (LOCAs), is paramount. In a LOCA scenario, where coolant leakage causes a rise in fuel rod temperature, the cladding may experience significant anisotropic deformation before ultimately rupturing—a phenomenon termed as 'cladding ballooning'. This type of deformation (depicted in the fig. 1) is especially dangerous, given how it restricts the coolant flow in the tightly packed fuel assembly, resulting potentially to a sequence of events in which multiple rods fail. To perform accurate safety analyses for fuel rods in these conditions, this anisotropic high temperature deformation needs to be modelled in state-of-the-art capability (1).

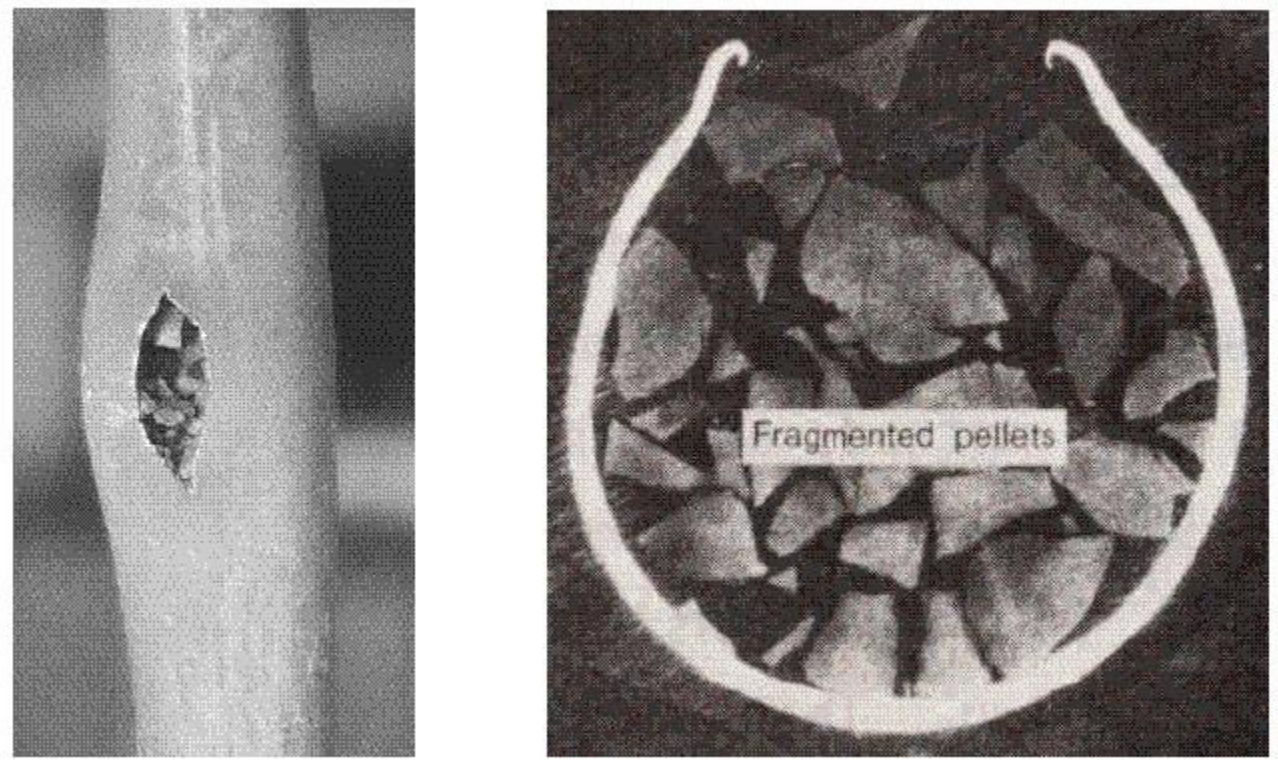

Figure 1: Example of a mechanical rod failure caused by ballooning (2).

To predict the transient thermo-mechanical behavior of fuel rods, fuel performance codes (FPC) are used for analyzing the intricate thermo-mechanical response of fuel rods. State-of-the-art examples of FPCs, such as the transient solver FRAPTRAN-2.0, have been capable of modelling LOCAs and ballooning phenomenon already for decades (3). Newer FPCs exist as well, such as the 3D BISON fuel performance code (4). These codes, generally based on finite element/volume/difference methods, have undergone validation against experimental data to ensure accuracy. They provide insights into nuclear fuel behavior and aid in developing new fuel rods.

VTT's in-house FPC FINIX, however, has not yet had a suitable high-temperature cladding deformation model implemented for LOCA modelling, and as such is limited in its function (5). In-house codes are often preferred, as they enable flexible development and coupling, and are valuable development targets in terms of competence building. As such, this work aims towards implementing the first working version of the relatively lengthy BALON2 ballooning module (1). BALON2 was chosen to be implemented as it is publicly available and widely applied as part of the FRAPTRAN fuel performance code. The model has been prepared for the U.S. Nuclear Regulatory Commission (NRC). The ballooning model will be added as a new module in the FINIX, and validated against Halden IFA-650 experiments 5, 6 and 7, in which LOCA conditions were artificially created for base irradiated sample rods with various cladding materials.

2. Model implementation

BALON2 model is implemented as its own structure in the FINIX source code, which becomes activated upon the effective strain threshold of the cladding being exceeded in an axial region of the fuel rod. Once this activation occurs, the code transitions from using the standard cladding mechanical model to only calculating cladding mechanical behavior with the ballooning model in the ballooning region. Ultimately, this model can predict whether the ballooning results in a failure. If a failure occurs, the code no longer attempts to solve the mechanical behavior of the rod. The whole implemented routine has been visualized in the flowchart in fig. 2. A brief description is also provided below, pinpointing FINIX-specific points of interest, future targets for development and possible challenges.

(A) The BALON2 ballooning model is initiated once the mechanical deformation threshold is exceeded. A simple criterion has been used so far: exceeding 5% of effective strain initiates the ballooning event. Alternative criteria are present in the literature, and FRAPTRAN-2.0 utilises a more complex set of criteria which necessitate the strain threshold criterion to hold over consecutive timesteps for the ballooning to continue.

(B) Extract input values from the existing FINIX data structures and store them in a workspace specifically dedicated to the ballooning calculation (workspace->balloon data structure). In this manner, the sub-nodalization of the ballooning axial node into 16 axial and 16 radial subnodes is performed, and the calculation shifts away from the usual nodalization FINIX uses outside this function. Values such as internal and external pressures, and gas gap temperature are taken from the results and boundary condition structures. When the BALON2 is called for the first time (parameter ‘nbncal’ changes from 0 to 1), the various data structures of workspace->balloon are given initial dummy values. At this point the anisotropic geometry of the ballooning cladding is first defined.

(C) Stress components and cladding radial dimensions are solved.

(D) Function of cladding equation of state (CKMN) is invoked to solve the maximum allowable timestep as a function of temperature, oxygen concentration, fast neutron fluence and cold work, returning strength coefficient, strain hardening exponent and strain rate sensitivity exponent which are used to calculate the timestep.

(E) Fuel temperatures are updated through simultaneous linear equations solver to reflect the changes due to the anisotropic dimensional changes. This stage was not included in the original BALON2 model and based on the few validation cases studied in this work had quite an insignificant role. Regardless, similar model is in FRAPTRAN-2.0, named SIMQ in FRAPTRAN. After this, the cladding temperatures are updated based on the heat transferred through gap and via radiation.

(F) Changes in effective fluence and effective cold work are solved for the time increment via CANEAL function. The changes are not significant over the small time increments used in the ballooning calculation, but the initial FINIX input values of fluence and cold work need to be ‘converted’ into effective values for the future calculation. In this sense, CANEAL needs to be invoked at least once to obtain the desired effective values. Like in FRAPTRAN-2.0, oxidation is not solved at this stage, although it could be if considered significant.

(G) The solved stresses are compared against existing burst stress threshold criterion included in FINIX. If failure occurs, FINIX exits the BALON2 model and no longer re-enters it. The current burst stress criterion is a function based on correlation for Zircaloy from Erbacher et al. (6) that provides values that are different to the CMLIMT function included in the original BALON2 model but are of the same scale. In future work, the implementation of CMLIMT function and other potential burst criteria could be studied.

(H) Function CANISO is invoked to solve the cladding anisotropy coefficients to relate the effective stress to stress components and effective strain to strain components.

(I) Function CSTRNI is invoked to solve the cladding strain as a function of true cladding stress, initial true cladding strain, time step size, cladding temperature, oxygen concentration, fast neutron fluence and cold work. After this has been solved, new dimensions, bending and shape are calculated for the ballooning node.

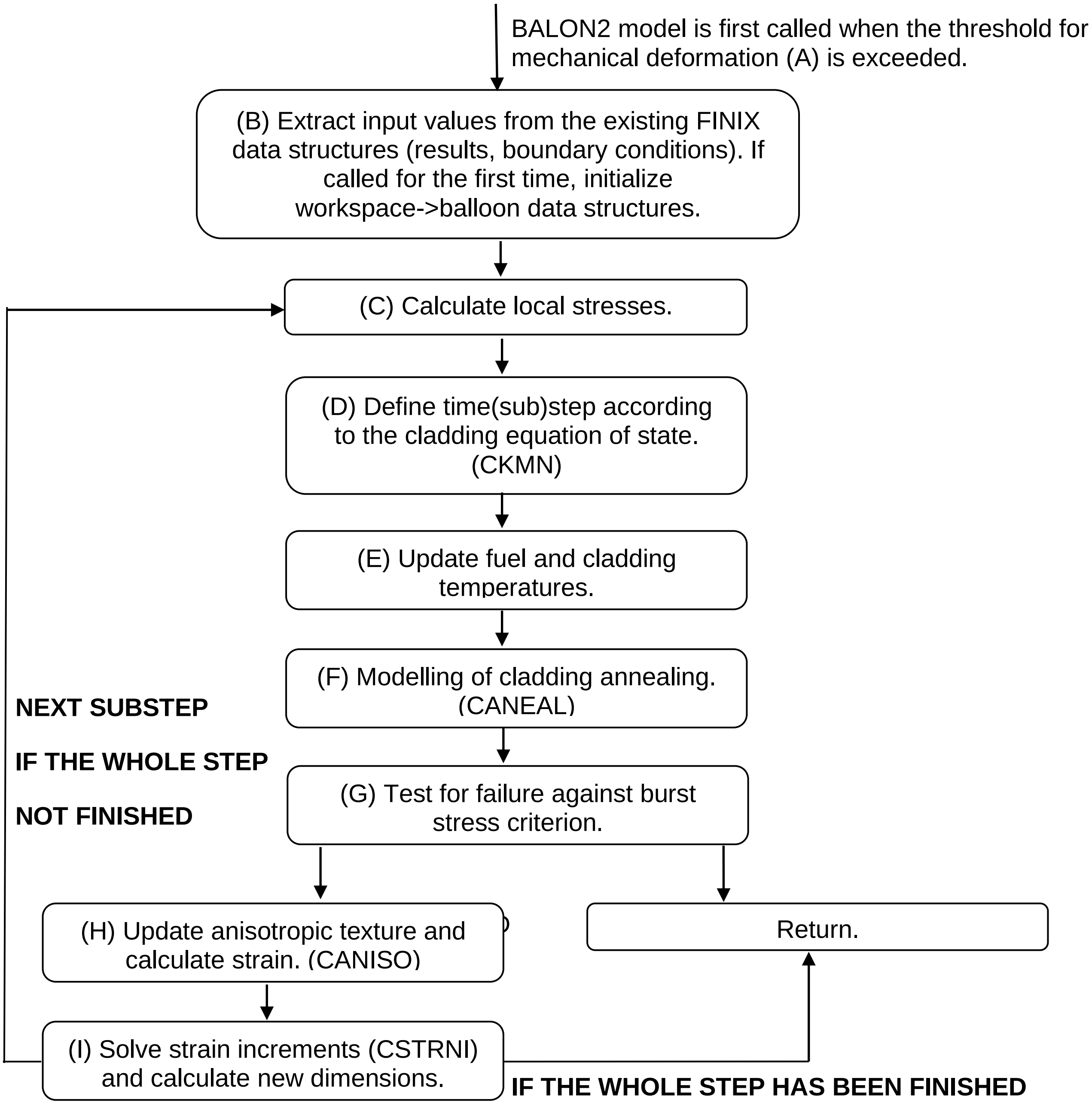

Figure 2. Flowchart of the implemented subroutines for modelling of the ballooning.

Functions (CKMN, CANEAL, CANISO, CNSTRI) called during the BALON2 model all originate from the publicly available MATPRO handbook (7) and have been included in the FINIX source code.

Although the core model of BALON2 was implemented to FINIX similarly to how it was included in FRAPTRAN-2.0, not all its details were included in this iteration. FRAPTRAN-2.0 calls BALON2 module through another module, FAR1, which in conjunction with the BALON2 model solves the coolant flow-area reduction resulting from the ballooning. This model was left outside the scope of this study due to prioritization, and due to the three validation cases all using a set cladding heat transfer coefficient as a boundary condition. For these cases, the heat transfer is not modelled dependent on the coolant flow, and consequently the FAR1 model was not considered relevant. Regardless, implementation of a model equivalent to FAR1 could be considered in the future as it benefits the internal thermal-hydraulics solutions in FINIX that solve the cladding-coolant heat transfer under certain given boundary conditions and options. The model could also have use in coupled calculations as a potentially valuable input data for a coupled thermal-hydraulics solver.

Similarly, future attention could be given to how FINIX handles fuel-cladding mechanics once the ballooning model activates. For FINIX, a simple condition was added to skip the standard cladding mechanics solver functions after the ballooning has initiated. FRAPTRAN-2.0, however, does perform some calculations in the non-ballooning mechanics functions as well. For FINIX this results in some parameters of interest not being produced as outputs. For instance, cladding permanent hoop strain is not an output as the final cladding radius includes also the thermal and elastic strain components at hot conditions even after the temperature has dropped after the transient.

3. Validation cases

For this work, three validation cases from the Halden IFA-650 LOCA experiments series were studied. These experiments were chosen on the basis of their status in the FRAPTRAN-2.0 integral assessment (8), which facilitates code-to-code comparisons and provides readily available input files for FRAPTRAN, in addition to those experiments already existing in the FINIX validation database. The relevant manufacturing and input parameters of the experiments are found for instance in (9).

FINIX calculation requires three input files (rod.inp, options.inp and scenario.inp), which define the rod parameters, calculation switches/options and boundary conditions, respectively. Additionally, in a transient calculation, a restart file is required to define the present burnup effects accumulated through the base irradiation of the IFA-experiments father rods. For this, FINIX can accept a FRAPCON-generated restart file. This restart file is the same file that is also used to initialize the FRAPTRAN transient LOCA calculation, to provide both codes a common starting ground.

Since the experiments were already included in the FINIX validation database of SPACE validation tool (VTT's in-house tool), the three input files and the restart file were printed through that tool and ran separately, after which they were post-processed using MATLAB plotting scripts. FRAPTRAN calculations were similarly run and relevant output was taken and included for the comparisons against FINIX through FRAPplot Excel tool.

Halden IFA-650 LOCA test series programme was active from 2003 until Halden's closure in 2020, with a dozen of experiments aiming to study LOCA behaviour of single fuel rods with varied claddings and generally high burnup. Experiments were set up to represent a low power level of fuel decay heat (few kW/m of linear heat) (10). These experiments were performed in both BWR and PWR conditions (with respective cladding materials), simulating the thermal boundary conditions with insulating channel and heated shroud, and a spray system for steam supply. Hoop strain experienced in the ballooning regions in these experiments ranges from 10% to 50+% (11).

Other relevant validation cases for future development could include other Halden IFA-650 tests such as the high burnup Zircaloy-4 fuel rods IFA-650-3 and IFA-650-4, as well as additional E110 validation case IFA-650-11. Furthermore, many additional validation cases remain in the FRAPTRAN-2.0 Integral Assessment, of which some could provide valuable examples of ballooned fuel rods that did not end up in failure. PUZRY high temperature ballooning and burst test data would similarly provide valuable additional scenarios for validation (12).

3.1 IFA-650-5

IFA 650-5 was a Halden LOCA test performed on a commercial PWR rod segment that had undergone six cycles of base irradiation up to the segment average burnup of 83.4 GWd/MTU. The rod was refabricated and refilled with helium-argon gas mixture up to the pressure of 4 MPa. During the experiment, the rod was placed inside a heated tube containing coolant that was removed to initialize the LOCA, after which spray was applied. The rod heated up steadily and the burst occurred at t = 179 s, with measured peak hoop residual strain of 16%.

The dimensions for IFA-650-5 calculation were obtained from the FRAPTRAN-2.0 integral assessment input files, which originally were based on the data sheet of the father rod. As mentioned previously, the base irradiation was not simulated in this work. Instead, a readily available FRAPCON restart file was taken from the integral assessment materials, which FINIX is able to read directly to establish the correct order of burnup effects at the start of the transient. A boundary condition of constant linear power (2.4 kW/m) is used alongside a given cladding outer surface temperature history ranging from 500 to 1300 K during the escalation of the LOCA. In this approach, the cladding surface heat transfer coefficient is given an arbitrarily high value (of 2e6 W/m^2 K), similarly to FRAPTRAN-2.0 reference calculations.

3.2 IFA-650-6

IFA 650-6 was a Halden LOCA test performed on a VVER rod segment that had been irradiated for four cycles at Loviisa nuclear power plant to a segment average burnup of 55.5 GWd/MTU. The rod was refabricated and refilled with helium-argon gas mixture up to the pressure of 3 MPa. As in IFA 650-5, the rod was placed inside a heated tube containing coolant that was removed to initialize the LOCA, after which spray was applied. The rod heated up steadily and the burst occurred at t = 525 s, with measured peak hoop residual strain of 36%

The dimensions for IFA 650-6 calculation were obtained from the FRAPTRAN-2.0 integral assessment input files, as with IFA 650-5. The base irradiation calculated on FRAPCON modelled the rod cladding as M5, as E110 was not an available option. Boundary conditions were applied similarly to the IFA 650-5 calculations, with constant linear heat rate value of 1.3 kW/m and cladding outer surface temperature ranging from 500 to 1100 K. FINIX has E110 correlations for some thermal and mechanical properties. However, these have not been widely tested and are not expected to cover all the relevant bases with some models using the same correlations for both Zircaloy and Zr1%Nb claddings. As a suggestion, this LOCA scenario could be revisited if E110 correlations in FINIX are studied further at some point.

3.3 IFA-650-7

IFA 650-7 was a BWR fuel rod segment that underwent base irradiation in the commercial Kernkraftwerk Leibstadt reactor for three cycles up to a segment average burnup of 44.3 GWd/MTU. The rod was simulated similarly to the other two IFA-650 cases, with a constant linear heat rate of 3.4 kW/m and coolant temperature ranging from 500 to 1500 K with an arbitrarily high heat transfer coefficient. The rod heated up steadily and the burst occurred at t = 247 s, with measured peak residual hoop strain of 24%.

4. Results

The results for each of the simulated IFA-650 LOCA scenarios are included in the subsections below. For each, the evolution of internal pressure is compared against experimental data and FRAPTRAN-2.0, while also assessing the time of ballooning initiation and rod burst.

With all the three rods, burst occurrence was predicted by both of the codes, which is also in alignment with the experiments. The initiation of ballooning differs between FINIX and FRAPTRAN-2.0, which is related to the differences in pre-ballooning mechanical calculation. The internal pressure evolves differently between the codes as well.

As mentioned at the end of Section 2, FINIX does not perform routines in the standard mechanical solution after the ballooning starts. Although this is not expected to play a significant role in the outcome of the ballooning and rod failure, currently the ballooning model in FINIX affects solely to the data structures of the BALON2 function, and as such the ballooned dimensions are not properly accounted for in the calls outside of that function. Consequently, the internal pressure is not calculated entirely correctly in FINIX and simply remains at a constant value once ballooning has started. This can be seen emphasized with a red circle in fig. 3. Feedback between the internal pressure calculation and the ballooning model could be a subject of future development, if more accurate modelling is pursued.

The shape of ballooned region was briefly studied for IFA 650-5 by comparing the cladding outer surface radial dimension at the last timestep prior to bursting for both FINIX and FRAPTRAN. This is mainly included (see fig. 4) to better understand the behavior of the ballooning model, as the solution provided by the model sometimes showcases non-physical behavior, such as with the zigzag-shape of FRAPTRAN's prediction in IFA-650-5. Lastly, in fig. 5, comparison of evolution of cladding maximum radius in FINIX and FRAPTRAN simulation is shown. It should be noted that with FINIX, the cladding radius is plotted here only during the ballooning as the pre- and post-ballooning radii have not yet been combined into a single output.

In FRAPTRAN-2.0's integral assessment, the maximum measured residual hoop strain is compared to the value found in the experiment. These residual values are significantly lower than the values obtained from FINIX as FINIX solution has the thermal and elastic components included. To be able to output the permanent strain could remain a topic of future work, which would necessitate revisiting the aforementioned relation between the standard mechanical cladding behavior function and ballooning model, with essential data transferred from the workspace->balloon structures into the data structures present in the standard solver.

4.1 IFA-650-5

For IFA 650-5, ballooning initiates at t = 101 s for FRAPTRAN, whereas for FINIX it initiates significantly later at t = 177 s. For FRAPTRAN this results in a failure at t = 170 s, whereas for FINIX the burst occurs at t = 184 s. The most notable difference here lies in the initiation and duration of the ballooning. Both codes provide a relatively good prediction of the timing of rod failure, with the in-experiment burst occurring at t = 179 s. In terms of the cladding radial shape, FINIX predicts a relatively flat radial profile with a relative maximum distortion of a few percents whereas FRAPTRAN predicts a non-physical zigzag-shape that has a peak radial value 25% higher than surrounding nodes. The codes predict the axial location of the maximum ballooning differently.

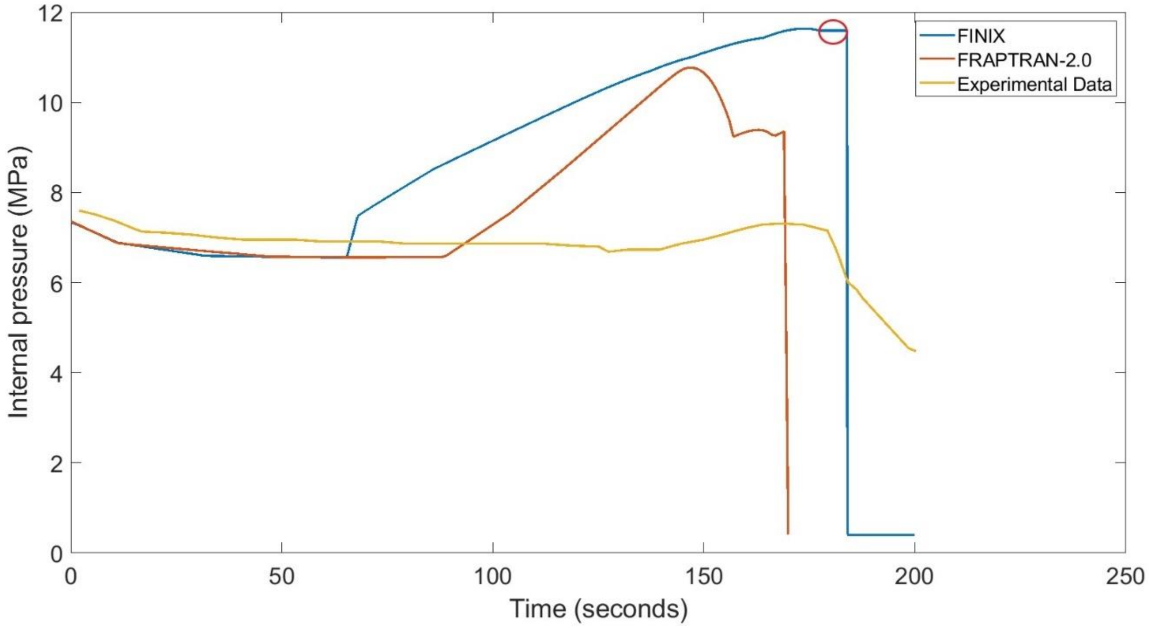

Figure 3: Comparison of rod internal pressure predictions and experimental results for IFA-650-5.

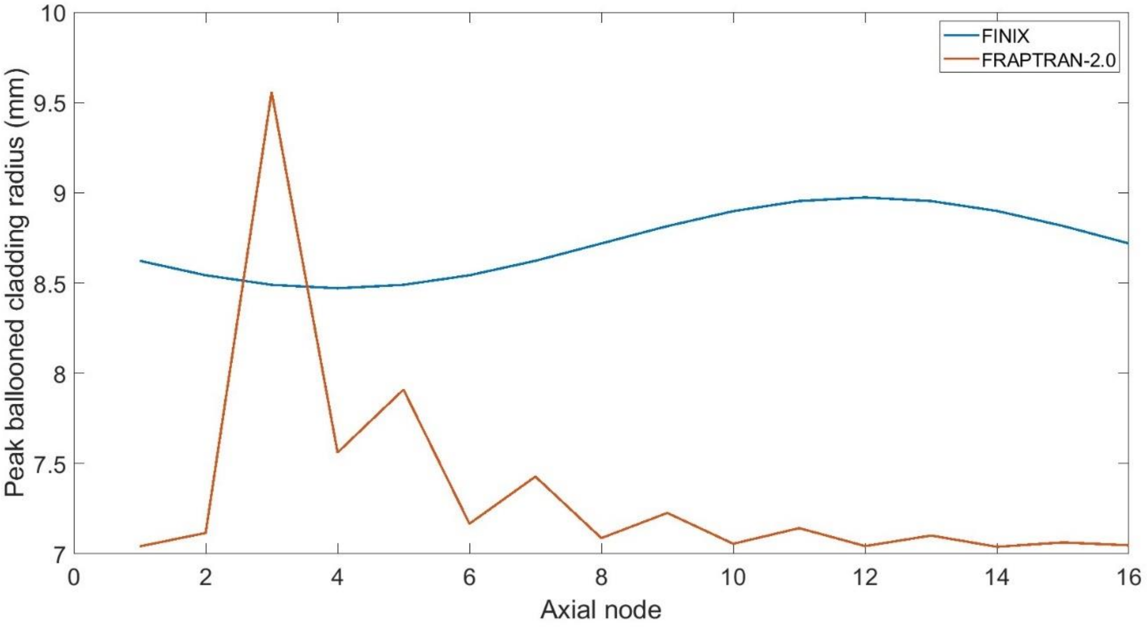

Figure 4: Peak cladding radius in the ballooning axial region prior to burst.

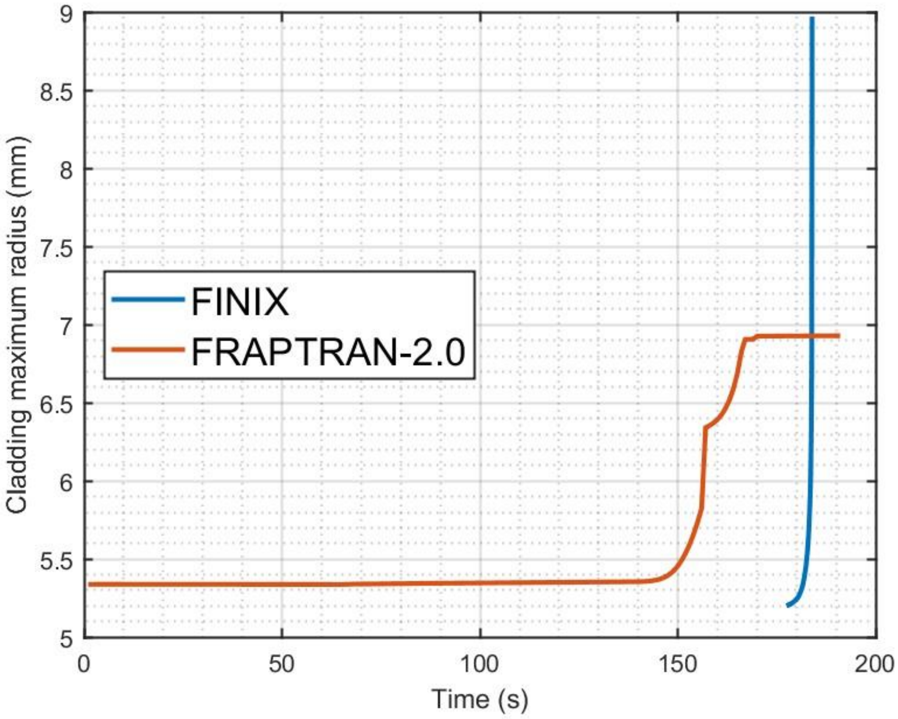

Figure 5: Peak cladding radius. With FINIX, the cladding radius is plotted here only during the ballooning.

4.2 IFA-650-6

For IFA 650-6, ballooning initiates at t = 359 s for FRAPTRAN, whereas for FINIX it initiates at t = 377 s. For FRAPTRAN this results in a failure at t = 419 s, whereas for FINIX the burst occurs at t = 401 s. Both codes predict similar sequence of events, with FINIX predicting higher initial pressure and earlier bursting, as can be seen from fig. 6. The actual burst occurred at t = 525 s, indicating that both codes underestimate the sturdiness of the rod. For FINIX this could be revisited with E110 correlations applied for burst criterion and other mechanical properties that lack proper correlations.

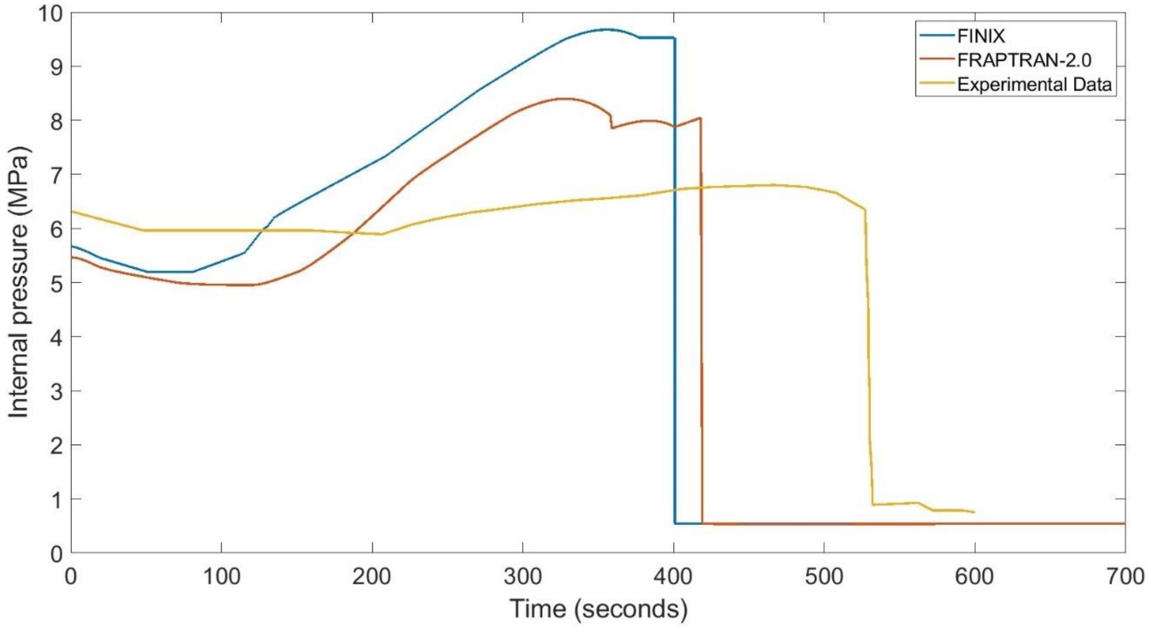

Figure 6: Comparison of rod internal pressure predictions and experimental results for IFA-650-6.

4.3 IFA-650-7

For IFA-650-7, ballooning initiates at t = 145 s for FRAPTRAN, whereas for FINIX it initiates at t = 87 s. For FRAPTRAN this results in a failure at t = 152 s, whereas for FINIX the burst occurs at t = 151 s, as can be seen from the fig. 7. Although both codes predicted a similar time for burst, the ballooning initiates in FINIX much sooner. The actual burst occurred at t = 247 s, indicating again that the codes predict the failure very conservatively.

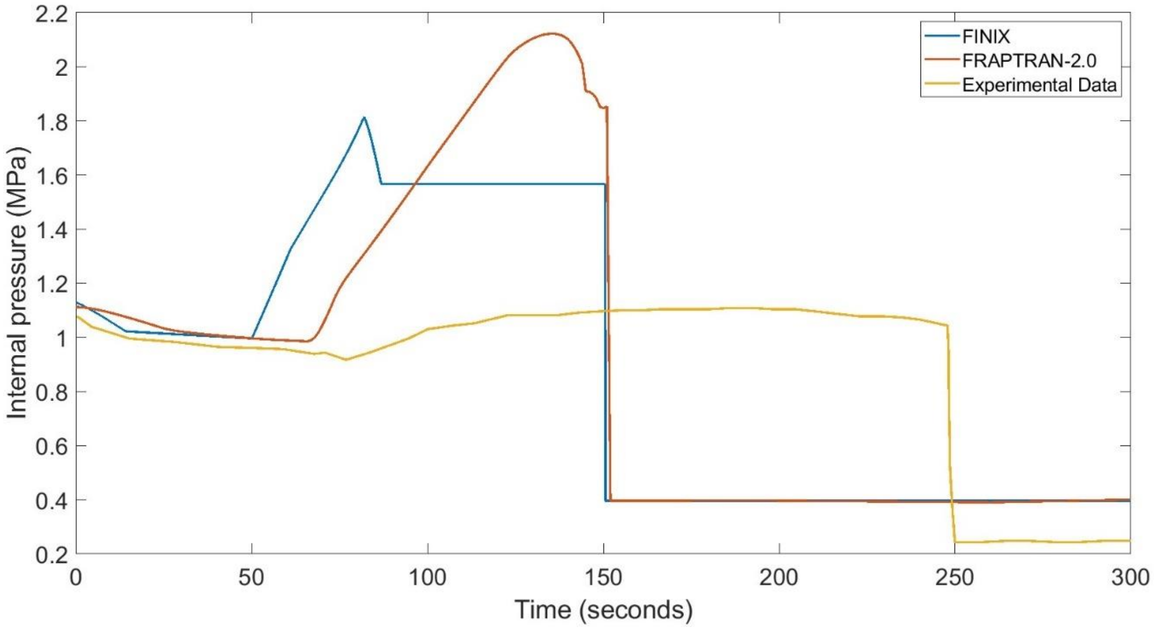

Figure 7: Comparison of rod internal pressure predictions and experimental results for IFA-650-7.

5. Summary and conclusions

In this work, publicly available cladding ballooning model BALON2 was implemented in VTT's in-house fuel performance code FINIX, to enable more realistic simulation of loss-of-coolant accident (LOCA) and other accident conditions in which anisotropic large cladding deformations can be expected to happen. BALON2 is the default ballooning model in widely used transient fuel performance code FRAPTRAN-2.0 by the U.S. NRC.

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FINIX does not yet provide estimates for residual cladding hoop strain, for which both experimental and reference calculation values exist for the purposes of code validation. This is related to fact that the coupling between the ballooning mechanics and standard mechanical solver are still missing. Furthermore, BALON2 model alone does not include all the tools for comprehensive modelling of effects of ballooning, such as models related to flow-area reduction.

This work succeeds in implementing the essential baseline model of cladding ballooning and enables the prediction of rod deformation and failure in LOCA conditions. Future work should be aimed towards finalizing the linkage between the BALON2 model data structures and the rest of FINIX, in order to provide estimates of residual hoop strain for further validation. Additional validation cases are available as well, and some parts of the code (such as burst stress criterion) could be revisited to further assess differences between FINIX and FRAPTRAN-2.0. The newly implemented LOCA model should improve the LOCA prediction capabilities of FINIX in coupled applications as well, although a thorough validation of FINIX transient modelling is advised prior to that.

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