

MODIFICATION OF TRANSURANUS FUEL PERFORMANCE CODE IN THE ATF FRAMEWORK

Alfredo Abe¹, Caio Melo², Claudia Giovedi³ and Antonio Texeira e Silva¹

¹Centro de Engenharia Nuclear – (CEN-IPEN/CNEN)
Instituto de Pesquisas Energéticas e Nucleares
05508-00 Av. Prof. Lineu Prestes 2242, São Paulo, Brazil
ayabe@ipen.br

²Centro Tecnológico da Marinha em São Paulo
Marinha do Brasil
05508-000 São Paulo, SP, Brazil
caio.melo@marinha.mil.br

³Analysis, Evaluation and Risk Manager Laboratory (POLI/USP)
Naval Engineering School - University of São Paulo
05508-000 Av. Prof. Mello Moraes, 2231
São Paulo, SP, Brazil
claudia.giovedi@labrisco.usp.br

ABSTRACT

The standard fuel system based on UO₂-zirconium alloy has been utilized on nearly 90% of worldwide nuclear power light water reactors. After the Fukushima Daiichi accident, alternative cladding materials to zirconium-based alloys are being investigated in the framework of accident tolerance fuel (ATF) program. One of the concepts of ATF is related to cladding materials that could delay the onset of high temperature oxidation, as well as ballooning and burst, in order to improve reactor safety systems, and consequently increase the coping time for the reactor operators in accident condition, especially under Loss-of-Coolant Accident (LOCA) scenario. The ferritic iron-chromium-aluminum (FeCrAl) alloys have been identified as an alternative to replace current zirconium-based alloys based on its outstanding resistance to oxidation under superheated steam environment due to the development of alumina oxide on the alloy surface in case of LOCA; moreover, FeCrAl alloys present quite well performance under normal operation conditions due to the thin oxide rich in chromium that acts as a protective layer. The assessment and performance of new fuel systems rely on experimental irradiation program and fuel performance code simulation, therefore the aim of this work is to contribute to the computational modeling capabilities in the framework of the ATF concept. The well-known TRANSURANUS fuel performance code that is used by safety authorities, industries, laboratories, research centers and universities was modified in order to support FeCrAl alloy as cladding material. The modification of the TRANSURANUS code was based on existing data (material properties) from open literature and as verification process was performed considering LOCA accident scenario.

1. ACCIDENT TOLERANT FUELS CONCEPT

Nowadays, ATF research and development program [1-6] involves efforts of different sectors from the international nuclear community including different universities, research institutes, regulatory authorities, and suppliers all around the world aiming to develop new fuel system which enhance safety in nuclear power plants. The main part of the researches that are being carried out is focused on the development and test of materials to be applied as cladding. These materials shall present good stability at high temperatures, especially in steam environment, in order to avoid the problem related to the hydrogen generation observed with zirconium-based alloys under accident scenarios. Despite of this, the material shall present low neutron absorption cross-section, good mechanical stability under irradiation, and feasible manufacturing process. According to recent NRC (Nuclear Regulatory Commission) document entitled: "DRAFT PROJECT PLAN TO PREPARE THE U.S. NUCLEAR REGULATORY COMMISSION TO LICENSE AND REGULATE ACCIDENT TOLERANT FUEL" [7], the ATF concepts can broadly categorized as evolutionary or revolutionary.

The evolutionary ATF can largely rely on existing fuel experience, material, models, and methods. Mostly are nuclear fuel designs such as coated zirconium cladding [8-12] and FeCrAl alloy [6,13-17]. The revolutionary ATF is related to fuel which has new type of fuel, cladding material, models, and methods that has to be developed to support the licensing process, such as U_3Si_2 fuel [18], metallic fuel, and SiC based cladding[19]. Considering ATF fuel system as two main components: fuel pellet and fuel cladding, for ATF fuel pellet concepts different than standard UO_2 are being suggested and investigated, especially material that can enhance thermal conductivity (high thermal conductivity) contributing to decrease the fuel temperature, reduce fission gas release, decrease thermal and mechanical stress. Moreover, high uranium density fuel is desired in order compensate some neutronic penalties that might be associated to proposed new cladding materials, avoiding the necessity of increasing the fuel enrichment level [20-24].

Concerning the cladding material, among different and promising candidates to be applied as cladding in ATF, many researches have been presented FeCrAl alloy as most suitable cladding as mid-term solution, FeCrAl alloys exhibits superior oxidation resistance under severe accident condition, moreover the formation of a chromium rich oxide layer on the surface under normal operation condition increase a protective coating in the cladding. Different studies on FeCrAl alloy materials have shown sufficient strength and ductility to perform acceptably as cladding alloy. The stiffness of FeCrAl is roughly twice that of Zircaloy [25], while the yield stress is higher by a factor of four [26]. Additionally, considering most of existing manufacturing processes used in zirconium alloy is similar and compatible for FeCrAl alloy cladding. There are some drawbacks and issues such as parasitic neutron absorption penalty (Fe neutron absorption is almost ten times higher than Zr) and potential increase of tritium [27] release in the primary circuit. The permeability of hydrogen in FeCrAl is about 100 times higher than its permeability in Zircaloy, therefore the main drawbacks shall be evaluated and find some reasonable solutions.

Nowadays, considering reliable and proven technology of cladding, the use of coatings material to improve current zirconium based alloy claddings is considering more promising and attractive approaches for ATF fuel cladding, the option can avoid major modification in the existing manufacturing process and also to become easier the licensing process. The addition of protective coatings in the existing cladding can prevent a severe oxidation and corrosion at high temperatures in the base material due to formation of a protective oxide on the surface [36]. This protective oxide layer used as coating shall be adherent and coherent, thick enough

and highly stable. The desired characteristics and requirements for protective coating are: capability to coat in existing cladding tube (zirconium based alloys) with attractive cost, minimal design changes in reactor core, low manufacturing temperature in order to avoid any changes in the microstructure of zirconium alloy, negligible neutronic penalty, appropriate and compatible thermal properties (high melting temperature) with zirconium alloy, improved corrosion, hydrogen pickup and irradiation resistance under normal operations, enhanced resistance to high-temperature environment (steam) under accident conditions, good mechanical properties and performance during accidental conditions (ballooning, creeping and cracking) [28]. The aim of this work is to modify TRANSURANUS fuel performance code [29] in order to address cladding material FeCrAl alloy and compare with standard zirconium based alloy.

2. FUEL PERFORMANCE CODE

The existing fuel performance and system codes [30-35] were mostly developed and validated for existing zirconium alloy cladding, currently limitations of the codes, data required and availability are being mostly identified in order to allow proper evaluation and assessment of ATF performance. In the last decade, many efforts have been made to improve simulation of DBA (Design Basis Accident) accidents such as LOCA considering coupled thermohydraulics and thermomechanics codes with fuel performance codes. Such system simulation codes mostly require detailed thermo-mechanical properties, correlations and models that has to be made available by means of specific experiments, in some cases, the proposed ATF fuel and cladding concept may be similar to the current fuel system, in such condition existing models and correlations can be applied with limited modification. However, cases in which the concepts of ATF fuel system deviate significantly from the current system, will necessarily require new development of material-specific models and correlations, that shall be tested and validated properly.

Considering the need of fuel performance code capable to perform evaluation and assessment of ATF, the well know TRANSURANUS code [29] was selected to be modified in order to consider FeCrAl as cladding material. The modification of the TRANSURANUS code is based on existing material data, thermo-mechanical model and correlation currently available for FeCrAl alloy.

The TRANSURANUS fuel performance code was developed at the Institute for Transuranium Elements (ITU). It consists of a clearly defined mechanical–mathematical framework, which new physical models and/or correlations can be easily implemented. Basically, the code is a simulation tool for the thermal and mechanical analysis of cylindrical fuel rods for nuclear reactors, that is used mostly by different universities, research institutes, nuclear safety authorities and industry. Basically, the code consists of a superposition of a one-dimensional radial and axial description, quasi two dimensional approach, where fuel rod is divided into axial zones and axial loop of calculation is performed taking to account zone by zone at given time, at end of calculation, all zones are coupled to obtain the macroscopic quantities such as internal fuel rod pressure and internal loading between cladding and fuel. Thermal and mechanical analyses are performed considering the data, correlation and models of different cladding and fuel. The code has a materials data bank for oxide, mixed-oxide, carbide and nitride fuels, zircaloy and steel claddings and different coolants. The scope of the covered phenomena and the numerical solution methods enables the code to simulate both long fuel cycles and design basis accidents. Moreover, options for sensitivity analysis is available in order to provide the possibility of a statistics based evaluation such as Monte Carlo simulations.

The code verification was based on: verification of the mechanical–mathematical framework comparing with exact solutions (analytical verification) when available, comparison with different solution techniques, extensive verification of models, code-to-code comparisons with many different codes and comparisons with experiments under steady state and accident conditions.

3. TRANSURANUS CODE MODIFICATION FOR FeCrAl ALLOY

The FeCrAl alloys is considered as more promising candidate for ATF cladding material, it is widely used in applications where low oxidation rates and high temperature performance conditions exist, primarily have been used as heating elements and components in high temperature furnaces due to their superior oxidation resistance over many other common materials. Over the past half a century FeCrAl alloys have also been considered for structural applications for varying industrial applications including for the nuclear power industry. Compared to traditional zirconium based claddings, FeCrAl alloys have higher strength and oxidation resistance, but a lower melting point and higher neutron absorption cross-section.

The thermal neutron absorption cross section of FeCrAl is about ten times that of Zircaloy, consequently the issue with FeCrAl cladding utilization is that the transition from Zr-based alloys to an Fe-based alloy will result in a neutronic penalty[21]. Therefore, thinner cladding walls, and slightly larger pellets with higher enrichment will be necessary to compensate for this neutronic penalty. The existing FeCrAl alloys span a wide range of compositions, microstructures and some alloying additions with different elements have successfully increased the strength of wrought FeCrAl alloys. Several commercial alloys are under consideration for nuclear applications but a vast array of studies had been completed on model alloys or simple alloy systems. Based upon the existing open and public data for FeCrAl (*Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications - ORNL/TM-2017/186 Rev. 1*) and empirical models, the TRANSURANUS code was modified.

Initially, the approach and guide to perform the TRANSURANUS code modification was based on existing stainless steel as cladding material, specifically the stainless steel AISI 316. The stainless steel AISI 316 models, correlations and data were identified inside of TRANSURANUS source code (written in standard FORTRAN 95), the subroutines or functions where such models, correlation and data were described. From the existing information of AISI 316 embedded in TRANSURANUS code as starting point to do the preliminary modification, the need of equivalent data, correlation and models for FeCrAl were identified and survey of such information was performed. The identified modification to be implement in the TRANSURANUS code is initially limited to some thermal and mechanical properties, therefore the modification assessment was not exhaustive in this work.

Following data, correlation and models were implemented: modulus of elasticity (ELOC), Poisson ratio (NUELOC), swelling (SWELOC), thermal strain (THSTRN), thermal conductivity (LAMBDA), creep rate (ETACR), yield stress (SIGSS), fracture strain (ETAPRR), true tangential stress at rupture of cladding as a function of temperature and oxygen concentration (burst stress) (SIGMAB), specific heat (CP), heat of melting (FH), emissivity (EMISS), Solidus and Liquidus Melting Temperatures (SOLIMT) and density (RO). The Figure 1 (extracted from: *Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications - ORNL/TM-2017/186 Rev. 1*) present a thermal expansion correlation implemented in the TRANSURANUS code. The fuel pellet data, models and correlations was kept as original, no modification was implemented in this work.

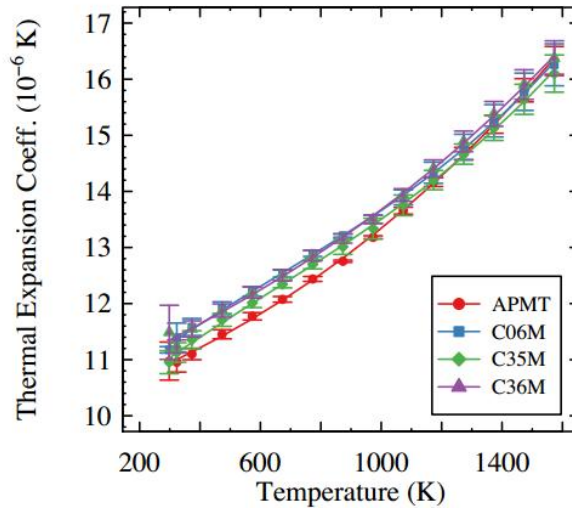


Figure 1: Thermal expansion model based on: *Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications - ORNL/TM-2017/186 Rev. 1*

4. TRANSURANUS CODE MODIFICATION ASSESSMENT

The TRANSURANUS code preliminary modification assessment was performed using experiment IFA-650.5 performed in the framework of Halden Reactor Project [36] to study the behaviour of $\text{UO}_2/\text{Zircaloy}$ fuel rod under LOCA scenario.

The IFA-650.5 test fuel rod was re-fabricated from an irradiated PWR $\text{UO}_2/\text{Zircaloy-4}$ fuel rod. The fuel had a high average burnup of 83 MWd/kgU. The base irradiation of the full-length rod comprised 6 reactor cycles corresponding to about 2000 effective full power days. The properties of the IFA-650.5 fuel rod are summarized in Table 1 below.

TABLE 1: FUEL ROD PROPERTIES OF IFA-650.5 TEST FUEL ROD

Fuel type	PWR
Fuel material	UO_2
Fuel pellet diameter (mm)	9.132
Fuel pellet length (mm)	11
Fuel dish depth (mm)	0.28
Fuel dish width (mm)	1.2
Fuel density (% TD)	94.8
Fuel enrichment (w/o %)	3.5
Cladding material	DX ELS0.8b
Cladding outer diameter (mm)	10.735
Cladding wall thickness (mm)	0.721
Fuel rod burnup (MWd/kgU)	83
Fuel rod total length (mm)	480
Fuel rod gap (mm)	0.0805
Fuelrodplenum volume (cm^3)	15
Fuel rod fill gas	90% Ar +10%He
Fill pressure (MPa)	4.0

The data from Table 1 were considered to build an input data for TRANSURANUS code, where the modified version (FeCrAl) was compared to original version with different fuel cladding (Zircaloy, E-110, AISI 316 and AISI 348). It is worthwhile to mention that the AISI 348 as cladding material is not part of original TRANSURANUS code, it was implemented by authors of this work as part of ATF program that are currently involved. The fuel rod was divided into 9 axial nodes, the radial fuel rod region was divided into 6 coarse nodes (5 for UO₂ and 1 for cladding), which each coarse node has 10 mesh. Moreover, different options (failure due to plastic instability or excess strain) of cladding failure were addressed in this preliminary assessment. The plastic instability is assumed if the effective creep rate was larger than 100 1/h and the effective creep was larger than 2 %, or clad failure is assumed when the radially averaged permanent true tangential strain exceeded a limit given by material property. The power profile considered was according to IFA-650-5 description and the temperature profile of fuel cladding was taken from experimental data available at IFA-650-5 documentation. Moreover, Heat transfer coefficient between coolant and fuel rod was set to infinity. The simulation was performed considering an equivalent 2000 effective full power days of burnup accumulation, before start the LOCA simulation.

5. MODIFIED TRANSURANUS CODE RESULTS

The assessment of modification implement was evaluate considering the simulation of IFA 650-5 experiment, moreover the results were compared to fuel rod cladding with zircaloy, E-110 (VVER), AISI 316 and AISI 348.

TABLE 2: Time of fuel failure (IFA-650-5 with different cladding material)

Cladding	Time of burst (sec.)
Zircaloy-4	76,75
E-110	74,71
AISI-316	84,06
AISI-348	85,95
FeCrAl	76,65

In this work, the time of burst is defined as time interval between beginning of the blowdown phenomena up to time of fuel rod experience any failure. The fuel cladding temperature profile after blowdown was taken from experimental data and heat transfer coefficient between coolant and fuel rod was set to infinity. According to obtained results, the FeCrAl exhibit similar fuel rod burst time compared to zirconium alloy (Zircaloy 4 and E110), the stainless steel cladding (AISI 316 and AISI 348) present slightly higher fuel rod burst time when plastic instability is considered as failure criteria. Moreover, when the radially averaged permanent true tangential strain is taken as failure criteria, the AISI 316 and AISI 348 experience failure almost immediately blowdown and others cladding material (Zircaloy 4, E110 and FeCrAl) fuel burst occurs due to the melting. It is worthwhile to mention that all time of burst obtained were always underestimate when compared experimental burst time (~178 sec.). The existing failure criteria of TRANSURANUS code shall play a very important role in simulation of LOCA accident.

6. CONCLUSIONS

The modification of TRANSURANUS code was performed in order to allow the assessment and analysis of FeCrAl cladding material performance. The verification of modification was made by means of IFA-650-5 experiment. The evaluated parameters of modified TRANSURANUS code was burst time of fuel rod with different cladding material. The results obtained shown that burst time obtained for different cladding material were underestimate when compared to experimental result. The main outcome of this work is the need to review the existing failure criteria of TRANSURANUS code. Moreover, it is important to mention that existing failure criteria adopted in different fuel performance code were developed for zirconium alloy cladding. In conclusion, this work contributes to identify limitation regarding fuel failure criteria for new ATF fuel cladding material.

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