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A REVIEW OF NUCLEAR FUEL PERFORMANCE CODES

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Abstract – The reliable prediction of nuclear fuel rod behaviour of nuclear power reactors constitutes a basic demand for safety-based calculations, for design purposes and for fuel performance assessments. There are many nuclear fuel performance codes, some of which are available in public domain. The recent fuel design and improvement activities are focused on to extend the burnup of fuel, and the use of new materials. Thus, the most important limitation of codes is the burnup validity limit. In this study, a review of the analytical capability of some of the existing computer codes for nuclear fuel performance calculations to highlight major strengths and weaknesses is performed.

Keywords – Nuclear fuel; fuel performance

1. INTRODUCTION

The reliable prediction of fuel rod behaviour of nuclear power reactors constitutes a basic demand for safety-based calculations, for design purposes and for fuel performance assessments. The ultimate goal of modelling is a description of nuclear fuel rod behaviour in both normal and abnormal operation conditions. From this knowledge, reactor operation rules can be derived to prevent fuel failures and the release of fission products to the environment by coolant or primary system and, in extreme cases, to prevent escalation of fuel and core damage and the consequential hazard.

It is also fundamental to the future of nuclear power that reactors can be run economically to compare with other forms of power generation. As a consequence, the development of the understanding of fuel performance and the embodiment of that knowledge in computer codes allow for more realistic predictions of performance. This in turn leads to a reduction in operating margins, and improved operating economics.

Fuel performance codes are important to help assure the continued safe operation of nuclear reactors that includes prediction the outcome of postulated accident situations. Thus, the fuel performance codes are

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interests of the reactor operators. Because of constantly increasing demands on reactor fuel efficiency (or increasing burnup targets), the development of new fuel rods with new materials and the reliability of these new fuel rods are interests of fuel vendors. Thus, the fuel performance codes are also important for fuel designer (or fuel vendor) to analyse the performance of this new fuel designs.

The real need of reactor operators and fuel vendors is to simulate nuclear fuel rod performance correctly. To accomplish this goal a minimum requirement is a well-proven fuel performance code. Since the codes required preparation of a detailed input data file, the simulation of a fuel rod with a well-established code requires an experienced simulation engineer.

The overall aim of the project is to develop an analytical capability to analyze the thermal and mechanical performance of commercial Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR) fuel by using well-proven public-domain codes and recently released fuel performance experimental data. This includes reviewing the available tools (i.e. codes) to generate experience on the use of the codes for different fuel performance problems and developing simulation experience on these codes, or improving the code if it is not fit for the problem requirements.

In this first part of the study, a review of the analytical capability of the existing computer codes for nuclear fuel performance calculations is performed to highlight major strengths and weaknesses of these codes.

2. CLASSIFICATION OF FUEL PERFORMANCE COMPUTER CODES

There are a number of available computer codes to analyse the thermal and mechanical behaviour of nuclear fuel rod of the different type of reactors (e.g. LWR, CANDU, VVER, etc.). However, in this study, only fuel rods of LWRs (i.e. PWR and BWR) are considered. Some of these codes are available in the public domain; for example, they can be obtained from OECD-Nuclear Energy Agency (NEA), while some companies have their own computer codes that are not available in the public domain.

The fuel rod behaviour is determined by thermal, mechanical, and physical processes such as densification, swelling, fission gas generation, fission gas release, and irradiation damage. Any fuel rod performance analysis code must include two parts: thermal and mechanical. The thermal and the mechanical parts include governing equations such as the heat conduction equation. Thus, the dimension of the equation is also an important parameter. In most of the fuel rod models, the theoretical and computational efforts are reduced by decreasing geometric dimensions. Although there are some 2-D and 3-D code developments, most codes are one-dimensional and are well developed and widely used. Then, the codes can be classified mainly as steady-state and transient codes.

The steady-state single-rod codes, like FRAPCON, TRANSURANUS, COMETHE, calculate thermal quantities such as radial temperature profile and fission gas release to the gap, and mechanical quantities such as creep deformation and irradiation growth. Results are used for many purposes like axial clearance between rods and end fittings, internal gas pressure to compare with system pressure, cladding oxide thickness to compare with established limits or to initiate transient calculations, stored energy for LOCA (loss of coolant accident) analysis and fission gas repartition between grains, grain boundaries and porosities for RIA (reactivity initiated accident) fuel failure mechanisms studies. These codes consist of models and correlations to describe gap conductance, material properties such as thermal conductivity and specific heat, radial power profiles, stress-strain equations, mechanical properties, creep properties, fuel swelling, fuel-densification, waterside corrosion, and hydrogen absorption.

The transient single-rod codes, like FRAPTRAN, also calculate thermal quantities and mechanical quantities. The range of models and correlations included in these codes is quite similar to that for the steady-state codes. The major differences between the transient and the steady-state codes are (a) the steady-state codes do not include transient heat-transfer terms in their solution equations, and (b) the transient codes do not include long-term phenomena like creep. However, the transient codes need to incorporate models, correlations, and properties for cladding plastic stress-strain behaviour at elevated temperatures, effects of annealing, behaviour of oxides and hydrides during temperature ramps, phase changes, and large cladding deformations such as ballooning. The mechanical description of the cladding

is two-dimensional ideally, but one-dimensional models are used as well. Other differences also come into models like fission gas release, which can have long-term and short-term components. The transient codes are used for analysing fuel rod response to transients and accidents like RIA and LOCA and may include failure models. In some cases, like fission gas release, the transient models would be quite different from the steady-state models. For burnup higher than 40-50 MWd/kgU, special attention should be devoted to the proper modelling of thermal characteristics of the so-called RIM-zone with its structural change and the consequent degradation of the fuel thermal conductivity. The phenomena of non-transient swelling and axial growth may not be modelled in the transient code because the transient time period is too short for significant non-transient swelling or axial growth. Different cladding materials and MOX (mixed oxide uranium/plutonium) fuel pellets will have similar effects as those described for the steady-state codes above.

3. REVIEW OF COMPUTER CODES

Table.1 lists the names of the fuel behaviour computer codes, with a short description that are distributed by the OECD-NEA Databank. Five computer codes for nuclear fuel performance calculations have been selected for preliminary evaluation. In the following subsections, a description of each of those codes is given.

3.1 FRAPCON-2/V1M4

FRAPCON series, like the earlier FRAP-S series, is designed to predict the steady-state long-term burn-up response of oxide fuel in light water reactors (LWRs). In addition, these codes generate the initial conditions for transient fuel rod analysis by the FRAP-T or RELAP codes. The first abstract of the FRAP-S1 was distributed in August 1976. FRAP-S2 was submitted in December 1976, and replaced in January 1979 by FRAP-S3 [1], replaced in November 1981 by Edition B, but deleted in December 1987. The Edition B of FRAPCON-1 [2] was submitted in December 1978, replaced by a revised edition in March 1979, replaced by a second revised edition in August 1980. Then, FRAPCON-2 was released in September 1980 [3]. FRAPCON-2/V1M2 and V1M3 were released in June 1981 and April 1982, respectively.

FRAPCON-2/V1M4 (abstract released in March 1983) [4] is the most recent in the FRAPCON series of fuel rod response modelling programs that is available at the NEA Databank. This version of FRAPCON (i.e. FRAPCON-2/V1M4) series has been modified and released as FRAPCON-2/V1M5B in January 1989. Idaho National Engineering Laboratory (INEL) and Battelle Pacific Northwest Laboratory (BPNL) have developed this code for the US Nuclear Regulatory Commission (NRC).

Some programming errors have been corrected in the versions of V1M2 and V1M3, and those corrections have been released in June 1981 and in April 1982, respectively. The letter dated Feb.7, 1983 describes the changes that have been made in the code in order to create FRAPCON-2/V1M4. The major modification to FRAPCON-2 is the new version of the FASTGRASS [5] fission gas release subroutine that has been included. The new version includes the effect of fuel micro cracking and hydrostatic stress upon the fission gas release mechanisms. The gap size iteration algorithm in the FRACAS-II subcode was altered; the iteration is now started at the hot unrelocated gap size, rather than at zero gap size. The power-time step was increased from 100 time steps to 200 time steps. Some corrections were made for the output the code.

FRAPCON-2/V1M4 calculates the temperature, pressure, deformation, and failure histories of a fuel rod as functions of time-dependent fuel rod power and coolant boundary conditions. The phenomena modelled by the code include heat conduction through the fuel and cladding, cladding elastic and plastic deformation, fuel-cladding mechanical interaction, fission gas release, fuel rod internal gas pressure, heat transfer between fuel and cladding, cladding oxidation, and heat transfer from cladding to coolant. Material properties, water properties, and heat transfer correlation data are included.

Table 1

Fuel Behaviour Computer Codes Distributed by the OECD/NEA Data Bank

Program Name	Description
ANSCLAD-1	Creep strain in fuel pin zircaloy clad during temperature transient
BUST	Elastic stress in HTGR pressurized fuel element
COMET	Mechanical & thermal stress in fuel element clad
COMTA	Ceramic fuel element stress analysis
DRUCK	Thermal - mechanical stress of PWR fuel rod during LOCA blow-down
FAMREC	PWR lateral mechanical fuel rod assembly response
FASTGRASS	Gaseous FP release in UO2 fuel
FEMAXI-V	Thermal & mechanical behaviour of LWR fuel rods
FRANCO	FEM fuel rod analysis for solid & annular configurations
FRAPCON2	Steady-state LWR oxide fuel element behaviour, FP gas release, error analysis
FRAP-T	Temperature & pressure in oxide fuel during LWR LOCA
FRETA-B	LWR fuel rod bundle behaviour during LOCA
FREVAP-6	Metal FP release from HTGR fuel elements
GAPCON-THERMAL3	Fuel rod steady-state & transient thermal behaviour - stress analysis
GRASS-SST	Fission gas release & fuel swelling in steady-state & transients
GAPCON-THERMAL2	Steady-state fuel rod thermal behaviour & FP gas release
HASSAN	Time dependent temperature distribution & stress & strain in HTGR fuel pins
LIFE-1	Stress analysis swelling, cylindrical fuel element performance in fast reactors
MARGE SLUMP	Radial temperature distribution & void diameter, MOX LMFBR fuel pin
MOXY/MOD-1	Thermal analysis swelling & rupture of BWR fuel element during LOCA
PIN99W	Modelling of VVER and PWR fuel rod thermal & mechanical behaviour
RODBURN	Power profiles & isotopics in PWR - BWR fuel rods (input for FEMAXI-V)
SPAGAF	PWR fuel, cladding behaviour with FP gas
SSYST-3	Modular system for transient fuel rod behaviour under accident conditions.
STOFFEL-1	Steady-state in-pile behaviour of cylindrical water-cooled oxide fuel rod
TAPIR	Thermal analysis of HTGR with graphite sleeve fuel element
TEMPUL	Temperature distribution in fuel element after pulse
THETA-1B	Fuel rod temperature distribution by 2-D diffusion, heat-transfer to coolant
WELWING	Material buckling for HWR with annular fuel element
WREM TWODEE-2/MOD3	2-D time-dependent fuel element thermal analysis after LOCA
ZZ FUELS-DATA	Data library for LWR fuel behaviour for FRAP program

3.1.1 Models of FRAPCON-2

In the fuel rod thermal response, the temperature distribution throughout the fuel and cladding is calculated at each axial node. The models used in the fuel rod temperature calculations assume a cylindrical fuel rod surrounded by coolant. The coolant inlet temperature, equivalent heated diameter, coolant mass flux, and axial linear heat generation rate, which are user-supplied parameters, are used to calculate the coolant bulk temperature, and then the film temperature rise is calculated from the coolant to

the surface of the fuel rod through any crud layer which may exist. In the calculation of film temperature rise, the Dittus-Boelter convection heat transfer correlation is used.

In the fuel rod mechanical response, the modelling of the cracked and relocated fuel, both thermally and mechanically, requires accounting for the changed fuel conductivity, the changed fuel-cladding gap size, and the changed fuel pellet diameter as the fuel interacts with the cladding. Two models are used to account for these phenomena: effective fuel thermal conductivity, and fuel surface relocation. The effective fuel conductivity model is a correlation that provides a multiplier on the MATPRO fuel conductivity. The fuel surface relocation provides a new fuel-cladding gap size for use in gap conductance calculations and mechanical interaction calculations.

FRAPCON-2 has three mechanical response model options: FRACAS-I, FRACAS-II, and PELET/RADIAL. FRACAS-I uses the effective fuel conductivity and the relocated fuel-cladding gap size for the thermal calculations but does not make use of the fuel surface relocation in the mechanics calculations. When FRACAS-I mechanics model is chosen, the fuel rod failure probability is also calculated. FRACAS-II uses the effective fuel conductivity and the relocated fuel-cladding gap size for the thermal calculations but unlike FRACAS-I, the relocated fuel surface is used in the mechanics calculations. The PELET/RADIAL mechanics model includes two parts: RADIAL model which estimates the thermal/mechanical state of the fuel during a time step, and PELET model which calculates the incremental elastic-plastic cladding deformation at the end of the time step. The PELET model is taken from GAPCON-THERMAL code.

Fission gas release in FRAPCON-2 includes these model options: ANS-5.4, Beyer-Hann (with NRC correction and without NRC correction), MacDonald-Weisman, and GRASS [6]. The ANS-5.4 gas release model is calculated as a function of time and fuel temperature and burnup. A user requirement is that the time step size be such that the burnup increments do not exceed 2000 MWd/MTU. Beyer-Hann gas release model identifies discrete constant release rates from three different temperature zones in the fuel. The NRC-recommended gas release enhancement factor for high burnup fuel (greater than 20000 MWd/MTU) has been added to this model. The NRC correction factor is a function of burnup. The MacDonald-Weisman gas release model considers the release determined by escape of gas from the fuel matrix and release of trapped gas from grain boundaries or dislocations. The GRASS gas release model is highly mechanistic gas release model, which accounts for bubble formation, migration, coalescence, and channeling and eventually release.

FRAPCON-2 uses MATPRO-11 for the material properties package. This package includes fuel and cladding material properties such as specific heat capacity, thermal conductivity, fuel swelling, densification, thermal expansion. The MATPRO-11 fuel thermal conductivity model calculates the conductivity as a function of temperature, density, oxygen to metal ratio, and PuO_2 content.

3.1.2 Solution Scheme of FRAPCON-2/V1M4

FRAPCON-2 iteratively calculates the interrelated effects of fuel and cladding temperature, rod internal gas pressure, fuel and cladding deformation, release of fission product gases, fuel swelling and densification, cladding thermal expansion and irradiation-induced growth, cladding corrosion, and crud deposition as functions of time and fuel rod specific power. The calculation begins with processing of input data. Next, the initial fuel rod state is determined through a self-initialization calculation. Time is advanced according to the input-specified time- step size, a steady state solution is performed, and the new fuel rod state is obtained. The new fuel rod state provides the initial state conditions for the next time step and these calculations are cycled in this manner for the user-specified number of time steps.

The solution for each time step consists of a calculation of the temperature of the fuel and cladding, a calculation of fuel and cladding deformation, and a calculation of the fission product generation, void volume, and fuel rod internal gas pressure. Each of the calculations is performed in a separate subprogram. The fuel rod response for each time step is determined by repeated cycling through two nested loops of calculations until the fuel rod temperature, deformation, and internal gas pressure converge.

FRAPCON-2/V1M4 is limited to single-rod analysis with 11 radial nodes in a pellet. It allows a maximum of 18 axial nodes and a maximum of 200 power time steps. The thermal models of the code are

based on steady-state data and equations; therefore, calculated temperatures will become progressively inaccurate as input power histories result in power ramp rates greater than 0.02 percent per second. Similarly, the gas release models are based on steady-state data and do not reflect release rates for rapid power changes. All the thermal and mechanics modelling options assume an axisymmetric fuel rod. Large deformations, with greater than 5 percent strain, will not be traced well. If the PELET option is selected, power step changes greater than 1.0 KW/ft per time step should not be used.

The code has been developed on a CDC CYBER 176 computer originally, however, the code has been tested on DEC VAX 6000 computer (i.e. operating system VMS) at NEA as well. The running time varies with the number of time steps and the number of axial nodes specified. Staff at the US National Energy Software Center (NESC) executed the FRAPCON-2/V1M4 sample problem in 195 CP seconds on a CDC CYBER170/875.

3.2 GAPCON-THERMAL-2 Rev.2 (GT2R2)

GAPCON-THERMAL-2 (GT-2) is an updated version of GAPCON-THERMAL-1 (GT1) [7] for calculating light water reactor fuel thermal performance. In general, GAPCON-THERMAL-1 has been modified to reduce uncertainties associated with the calculation of power history and burnup. Then, GAPCON-THERMAL-2 was released on November 1975 [8]. The GT2R2 [9] is the Revision-2 of GAPCON-THERMAL-2. It contains a number of coding corrections and updates, and now conforms to the American National Standard Institute (ANSI) FORTRAN-77 standard. The manuscript of GT2R2 was published in September 1984. The NEA distributes GT2R2-1.

GAPCON-THERMAL-2 calculates the thermal behaviour of a nuclear fuel rod during normal steady-state operation. The program was developed as a tool for estimating fuel-cladding gap conductance, temperatures, pressures, and fuel-stored energy. Models used include power history, fission gas generation and release, fuel relocation and densification, and fuel-cladding gap conductance.

3.2.1 Models of GT2R2

In the power history simulation, the code uses constant power for each finite time step. The power history dependent models in the code are fission gas release, relocation and densification. At any time step other than the first for each axial node, the current fission gas release, relocation and densification values are compared with the values used in the previous time step. Relocation and densification displacements will not decrease if lesser values are subsequently calculated. The fission gas release algorithm depends on all previous fission gas release values.

The fission gas (krypton and xenon) generation model has been modified by Carter [10], and is given in Ref.[8]. The mathematical model for fission gas generation in GT2 does not require that time starts at zero. Another addition in the new model includes the transmutation to plutonium of uranium-238 by resonance absorption of neutrons and subsequent gas production from fissioning of this plutonium.

The model in the subroutine of GT2 is based on linear regression analysis of experimental data. The model describes the increase in fuel diameter as a function of power (kW/ft), the as-fabricated cold gap thickness (inches), and burnup (MWd/MTM).

The fuel densification correlation in GT2 calculates the reduction of the fuel radius as a function of burnup (maximum 2000 MWd/MTM) and differential fuel density. Because no radial expansion is permitted, if the calculated value is greater than zero, it is set equal to zero.

The gap conductance is composed of three terms: conductance through points of contact (h_{solid}), conductance through the gas (h_{gas}), and conductance by radiation from fuel to cladding ($h_{radiation}$). The first term contributes only after contact has occurred if the contact is not due to relocation. The correlation developed from the data of Ross and Stoute [11] calculates the h_{gas} as a function of contact pressure, gas temperature, and surface roughness. The measured and the calculated values of the h_{gas} have been compared by linear regression again. Then, the constants in the expression of the correlation for h_{gas} have been modified slightly for the before-contact and after-contact cases to produce a continuous function. The term h_{solid} is calculated by the Mikic-Todreas model [12]. This modified model ties together the data of Raphier [13] and Ross-Stoute [11].

For the fission gas release, high and low temperature models included in GT2 were developed to provide an improved method for predicting gas release from UO_2 fuel. The high-temperature (> 1200°C) release model [14] was fitted to a consistent and well-characterized set of 45 data points using a multiple-linear regression code. The low-temperature (< 1200°C) gas release model proposed by Bellamy and Rich [15] was modified for use in GT2. The modification is only done on the surface-to-volume ratio which is one parameter of the gas release model.

A study was made on the fuel volatile impurity release rates and the subsequent reaction rates of these gases with the cladding. The result of this study was used in GT2 to model the behaviour of hydrogen, moisture, nitrogen, CO_2, and CO. The total quantity of sorbed gas and the mole fraction of each gas are input data. Notably, the impurity release rates are not calculated. The reaction rates of nitrogen and carbon monoxide that react with the zircaloy cladding are calculated.

The GT1 code does not consider fuel dishing. To improve the accuracy of the calculation of internal pin pressure, a simple algorithm for pellet dishing was included in GT2. Dish volumes are approximated by a void in the form of a short cylinder with the radius of the dish being the radius of the cylinder. The GT2 considers one dish per axial segment. The amount of dish volume available in the fuel column is to be input in terms of percent fuel column volume, and the radius of the dish.

The properties of the code for considering recycle mixed-oxide fuel below ~5 wt% PuO_2 are the same as those for UO_2 except for theoretical density, thermal conductivity and melting temperature. The GT2 includes a model to accommodate analysis involving molten fuel. Based on the fuel melting temperature the melt radius is calculated using the radial temperature profile. Next the volume of molten fuel is calculated followed by the volume of porosity available from the melt assuming the molten fuel is 100% dense. The gas release model assumes 100% release from the molten fuel of the generated fission gases.

The sum-of-nodes method for fuel radial thermal expansion [16] has been added as an option. This method assumes a number of rings of equal width and then sums the thermal expansion of each ring. Another fuel relocation model [17] has been added to the subroutine RELOC as an option. This model is a simple function of linear heat generation rate and burnup. The subroutine CREEP has been added to the code. CREEP incorporates the BUCKLE equations [18] for calculating cladding creepdown. The model calculates cladding creepdown as a function of external coolant pressure, rod internal gas pressure, cladding texture factor, cladding cold work, neutron flux, and time. Using the cladding creepdown calculation is optional.

A subroutine named RADAR was added to calculate the burnup dependent fuel radial power profile for each axial node. The model is the model [19] of the RADAR code developed by British Nuclear Fuels Ltd. The subroutine VOIDP was also added to calculate void fraction in case of BWR. The radial power distribution is calculated as a function of fuel design, burnup, and coolant void fraction. The user can enter the radial power distribution as well.

The GT2 code was originally developed using the Beyer-Hann fission gas release model [14]. This model was then modified with the NRC correction [20]. A major addition to GT2R2 is the ANS-5.4 fission gas release model [21]. The diffusion coefficient used in ANS-5.4 has been modified [22], and this has been added to the code as another option.

3.2.2 Solution Scheme of GT2R2

The GT2R2 calculates the gap conductance, temperatures, pressures, and stored thermal energy in a nuclear fuel rod. The code calculates these values for a fuel rod during its operation following its power history. The current version uses 50 fuel radial nodes and between 1 and 20 axial fuel nodes for as many as 35 time-power steps.

The fuel to cladding gap conductance for each equal-length, user-designated axial region is determined by an iterative scheme. Radial temperatures are calculated using a finite difference procedure. The solution procedure consists of iterative convergence for each axial fuel region, followed by iterative convergence on the fuel rod gas release for each time-power step. Empirical, theoretical, and physical models are used for the fuel gas release that is explained above.

The coding has been made ANSI-FORTRAN 77 standard (except for INCLUDE statements). Rod average burnup is now printed for each time step and has taken the place of stored energy in the summary page. Most models have been compared individually with experimental data; however, the code as a whole has not been adjusted to conform any to any set of data. Typical run time on the CDC CYBER74 is approximately 30 seconds per time-step; the sample problem runs in less than 20 CPU seconds on a CDC7600.

3.3 PIN99W

The PIN-micro code has been developed by Nuclear Research Institute, Rez, plc. of Czech Republic in 1982 [23], and its 1990 version was transferred to the OECD-NEA Data Bank in 1991 [24]. The PIN99W code [25] is an updated and improved version of the PIN-micro code, and it is available at the NEA Databank as well. The code has been used at both NRI (Czech Republic) and RRC "Kurchatov Institute" since 1991.

The PIN-micro computer code is based on the GAPON-THERMAL-2 methodology. The code is developed to describe fuel rod thermo-mechanical behaviour in operational conditions. The main goal of this code is to calculate fuel temperature, gap conductivity, fission gas release and inner gas pressure under steady-state conditions. The code involves models describing physical phenomena typical for the fuel irradiated in Light Water Power Reactors such as densification, restructuring, fission gas release, swelling and relocation. The code can be used for PWR and VVER fuel rods. Some models have been removed from the code such as: zone empirical model of the gas release taken from GT2 code, models for fuel swelling from GT2 code, and gap conductivity from FRAP code. The coding has been changed to standard FORTRAN-77. It can be run on a PC with Windows 95/98/NT operating system and Lahey FORTRAN-77 compiler.

3.3.1 Models of PIN99W

The empirical correlation for fuel relocation with new constants obtained during the FUMEX program was optionally added for fuel relocation [26]. Those constants are 42 and 0.9 for the GT2 option, and in this new option they are given as 14 and 2.7, respectively. However, the GT2 option is still recommended by the authors of the code.

The code has four correlations for fuel thermal conductivity calculations: Lyons (i.e. GT2 correlation), Kolyadin, Kajer-Pederson, and Wiesenack correlations. Only the Kayer-Pederson and Wiesenack correlations include the conductivity degradation with burnup. The Wiesenack correlation is recommended by the code authors.

The new neutron flux depression model permits separate calculation of the radial power density and burnup, as a function of the pellet geometry, enrichment and the average pellet burnup. The number of nodes is set by the user only. The radial power density and burnup profiles are not introduced by externally (i.e. by the user).

At burnup higher than 60 MWd/kgU, formation of a so-called RIM-region at the pellet periphery begins and is characterized by sub-micron grains and an increased porosity [27]. The newly added method calculates gas release from the RIM-region [28]. This model is applicable for burnup greater than 55 MWd/kgU.

An empirical expression is used to calculate the width of the RIM-region, and an empirical correlation is added to account for the increased porosity of the RIM-region.

3.3.2 Solution Scheme of PIN99W

The steady-state fuel rod temperature response is calculated by a one-dimensional finite element method combined with a weighted residuals method. The code has been tested against the SOFIT experiments data, and the data of the fuel rods irradiated at Kola NPP. For future work, the authors recommend including into the code a new gas release model, to innovate input possibilities for better thermal-hydraulic boundary condition treatment, and to update source code programming and improve the graphic interface.

3.4 FEMAXI-V (Ver.1)

A light water fuel analysis code FEMAXI-V(Ver.1) [29] is an advanced version which has been produced by integrating FEMAXI-IV(Ver.2), high burnup fuel code EXBURN-I, and a number of functional improvements and extensions, to predict fuel rod behaviour in normal and transient (not accident) conditions. The previous versions of FEMAXI-V are FEMAXI-III [30], FEMAXI-IV [31][32][33], and FEMAXI-IV(Ver.2) [34]. The series of FEMAXI codes are developed by Japan Atomic Energy Research Institute (JAERI). Here, the code description is summarized from Ref. [29].

FEMAXI-V (Ver.1) predicts the thermal and mechanical behaviour of a light water reactor fuel rod during normal and transient (not accident) conditions. It can analyze the integral behaviour of a whole fuel rod throughout its life as well as the localized behaviour of a small part of a fuel rod. Temperature distribution, radial and axial deformations, fission gas release and inner gas pressure are calculated as a function of irradiation time and axial position. Stresses and strains in the pellet and cladding are calculated and PCMI (pellet cladding mechanical interaction) analysis is performed. Also, thermal conductivity degradation of pellet and cladding waterside oxidation are modelled. Its analytical capabilities also cover the boiling transient anticipated in BWR. Elasto-plasticity, creep, thermal expansion, pellet cracking and crack healing, relocation, densification, swelling, hot pressing, heat generation distribution, fission gas release, pellet-cladding mechanical interaction, cladding creep and oxidation are modelled by the code. Efforts have been made to improve the numerical accuracy and stability of the transient analysis.

3.4.1 Models of FEMAXI-V

FEMAXI-V(Ver.1) integrates and extends the capabilities of the former version a FEMAXI-IV, which is applicable to middle burnup regions (more than 40 MWd/kgU), and EXBURN-I, a modification of FEMAXI-IV to cover high-burnup regions by incorporating new models. EXBURN-I was developed on the basis of FEMAXI-IV to analyze the problems specific to high-burnup regions, though the code did not include some functions of FEMAXI-IV(Ver.2). Therefore, FEMAXI-V has been developed to inherit and integrate all functions and capabilities of FEMAXI-IV(Ver.2) and EXBURN-I.

FEMAXI-V analyzes changes in the thermal, mechanical and chemical states of a single fuel rod components and their interactions in a given power history and coolant conditions. The analytical scope of FEMAXI-V covers normal operation conditions and transient conditions as well as load-following and rapid power increase, and also boiling transition of BWR fuels. However, it does not cover such conditions as LOCA.

The code includes a heat transfer to coolant and thermal-hydraulics model, a one-dimensional temperature calculation model, and a heat generation density profile model. As for material properties, several correlations are taken from the open literatures, and they are included into the code as options. For example, 12 correlations are given for UO_2 pellet thermal conductivity; four correlations are given for pellet thermal expansion. With respect to MOX fuel and Gd-contained UO_2 fuel, a rough calculation is possible by designating some of materials properties because the material properties for MOX and Gd-contained UO_2 fuel are used mainly the material properties correlations for UO_2 fuel with a correction factor. Thus, if an accreted evaluation is required for MOX fuel, this option of the code is preferably not used.

3.4.2 Solution Scheme of FEMAXI-V

FEMAXI-V consists of two main parts: a thermal analysis for analysing the temperature distribution, the thermally induced deformation, and the FP gas release; and the mechanical analysis for the mechanical behaviour of the fuel.

In the thermal analysis, calculation always covers an entire length of a fuel rod, which is divided into a maximum of 12 axial segments. In other words, the temperature distribution is calculated as a one-dimensional axisymmetrical problem in the radial direction, and with this temperature, such temperature-dependent values as FP gas release, gap gas flow in the axial direction, and their feedback effects on gap thermal conduction are also calculated. Within this thermal part, a simple mechanical model is used to

calculate such geometrical condition for temperature calculation as the deformation of pellet and cladding, and change in pellet-clad gap width. Accordingly, there is an iteration process between calculations of the temperature and temperature-dependent values, and calculation of the rod geometry obtained by the simple mechanical model to attain convergence at the end of each time step. Also, to deal with the thermal feedback among the axial segments, which may arise due to uneven power distributions in the axial direction, another iteration is performed until convergence is attained for the entire length of the rod.

In the mechanical analysis part outside the thermal analysis part, users can select either analysis of the entire length of a fuel rod, or analysis of one pellet length. In the first one, the axisymmetrical finite element method (FEM) is applied to the entire length of the rod; in the second one, the axisymmetrical FEM is applied to half of the pellet length (for reasons of symmetry), and mechanical interaction between pellet and cladding, i.e. local PCMI is analyzed. The magnitude of pellet strain caused by thermal expansion, densification, swelling and relocation are calculated first, and a stiffness equation is formulated with consideration given to cracking, elasticity/plasticity and creep of pellet. Then, stress and strain of pellet and cladding are calculated by solution of the stiffness equation with boundary conditions corresponding to the pellet-cladding contact mode. When PCMI occurs and states of pellet-cladding contact change, the calculation is restarted with the new boundary conditions of contact from the time when the change occurs. In the analysis of the entire length of a fuel rod, the axial force acting on an adjacent segment is evaluated and, as a result, an analysis of the axial deformation of entire rod length is performed.

Since temperature and deformation distributions obtained from the thermal and mechanical analysis parts physically depend on each other, simultaneous equations of thermal conduction and mechanical deformation should be solved. For instance, in order to obtain the temperature distribution of a rod, gap width should be determined by the mechanical analysis to calculate gap thermal conduction. So, coupling of the thermal analysis with the mechanical analysis by a convergence calculation loop is required. Therefore, the simple mechanical model that can determine the rod geometry within a short time is favoured to facilitate the time-consuming iteration process.

On the other hand, it is unrealistic to perform detailed stress/strain and displacement analysis within a short time, though it is the original objective of the mechanical analysis component. To avoid this contradiction, the mechanical analysis of the code has two independent parts. One is the simple mechanical model included in the thermal analysis to solve simultaneous equations of the temperature and deformation, and the other is a detailed mechanical analysis that is used for an accurate prediction of stress/strain and displacement distribution on the basis of the temperature obtained in the thermal analysis. These two mechanical analysis parts use common material properties and empirical equations.

Power profiles and burnup profiles in the radial and axial directions of a pellet vary with burnup from its early stages. This variations depends on the type of reactor; i.e. PWR, BWR, and heavy water reactor (HWR). Obviously, the temperature distribution of a pellet, and some material properties depend on the shape of these profiles. Therefore, similar to EXBURN-I, FEMAXI-V has a function to couple with the burning analysis code RODBURN. With RODBURN, profiles of power generation, amount of fissile materials in pellets, and fast neutron flux are calculated in accordance with the power history and fuel rod specification given, and a results file is generated. FEMAXI-V can read the data in this file for one of calculation conditions. RODBURN is also available at NEA (see Table.1).

3.5 FRAPCON-3

In recent work in the US, FRAPCON-3 has been developed. It is a computer code used for steady state and mild transient analysis of the behaviour of a single fuel rod under near-normal reactor operating conditions. FRAPCON-3 is a descendent of earlier GAPCON-THERMAL, FRAP-S, and FRAPCON-2 computer codes developed for the Nuclear Regulatory Commission (NRC) by the Idaho National Engineering Laboratory and the Pacific Northwest National Laboratory. Three volumes code manuals were released in 1997 [35] [36] [37], and the material properties have been taken from the MATPRO of RELAP5/MOD3.1 [38].

FRAPCON-3 models the thermal and mechanical behaviour of a fuel rod, and the code has been validated for burnups from 0-65 GWd/MTU (rod average). Previously the code (i.e. FRAPCON-2) had been validated up to about 40 MWd/kgU.

3.5.1 Models of FRAPCON-3

Fuel rod material properties and performance models have been updated for the FRAPCON-3 to account for changes in behaviour due to extended fuel burnup.

The FRAPCON-3 code has a new two-stage fission gas release (FGR) model. The model was originally developed by Forsberg and Massih [39] where the first stage quantifies the rate of grain-boundary gas accumulation due to diffusion and the concentration levels corresponding to saturation, and the second stage, the kinetics of grain-boundary gas release. Modifications have been made to the model diffusion coefficients with a burnup enhancement term added, and the resolution rate increased to predict high-burnup FGR from fuel rods with both steady-state power and power-bumping operation. The PARAGRASS [40] FGR model has been removed because it under-predicts FGR at moderate to high-burnup levels, and the ANS-5.4 [41] model has been retained because it predicts high-burnup FGR reasonably well for fuel rods operating at steady-state powers. It can calculate the release of volatile radioactive fission products such as iodine, cesium, and tellurium, in addition to xenon and krypton.

The MATPRO [38] model for fuel thermal conductivity has been modified to include degradation due to burnup and gadolinia additions based on out-of-reactor simulated, irradiated fuel diffusivity measurements and in-reactor centreline temperature measurements in high-burnup fuel. These changes will help to evaluate commercial fuel operation at higher burnup levels. The conductivity formula for sintered stoichiometric uranium dioxide as proposed recently by Lucuta et al.[42] has been evaluated and incorporated in FRAPCON-3 in place of the MATPRO-11 function of temperature and porosity. This formula includes the effects of temperature, radiation (environment), fuel burnup, and porosity. A modification for the effect of limited gadolinia additions has been added by Pacific Northwest National Laboratory, and a modification for limited plutonia additions has also been added.

The MATPRO model for fuel swelling has been modified. Experimental evidence has suggested that the FSWELL solid fission product-induced swelling rate should be increased. The present solid fission product-induced swelling rate ($\Delta V/V$) in the MATPRO subroutine FSWELL is 7.74E-9 per MW-s/kgU for 95% TD fuel, which corresponds to 0.669% per 10 GWd/MTU. Estimates of the solid swelling rate have been derived from density stack elongation measurements from instrumented fuels tests in the Halden Reactor at about 1% $\Delta V/V$ per 10 GWd/MTU. Fuel pellets irradiated in commercial PWRs to pellet burnups ranging from 20 to 70 GWd/MTU have been measured for density. The estimated swelling rates range from 0.7 to 1.0 % $\Delta V/V$ per 10 GWd/MTU. Swelling due to fission-produced gas is not significant at the low fuel temperatures for normal commercial fuel operation to which FRAPCON-3 will be applied, and it has been removed from the swelling model.

The fuel cracking and relocation algorithms in FRAPCON-3 have been modified. The option for no crack factor reduction in the pellet thermal conductivity has been retained in FRAPCON-3. The best estimate pellet relocation model developed for GT2R2 has been modified for use in FRAPCON-3 in conjunction with the FRACAS-I (a subroutine of FRAPCON-2) mechanical model. In conjunction with the FRACAS-1 model, the original FRAPCON-2 used a lower-bound version of the GT2R2 model for gap closure due to relocation [9]. This model resulted in very large overestimates of BOL fuel temperatures for the standard IFA-432/513 cases, of the order of 100 to 200 K. This best-estimate GT2R2 relocation model was altered slightly to provide a best estimate prediction of fuel temperatures for FRAPCON-3. This GT2R2 model is a function of LHGR and burnup that is similar to Oguma's model [43], but less complex in form. The gap closure due to relocation as a fraction of the as-fabricated pellet-cladding gap is given.

The power and burnup radial distribution functions in FRAPCON have been modified. A model developed by Lassmann and colleagues [44] at the Institute for Transuranium Elements improves on the original RADAR subroutine for light water reactor applications. Both contain an exponential distribution function that governs the radially dependent buildup of the plutonium and effective cross-sections for the plutonium and uranium isotopes. In order to install and use the TUBRNP sub code, the FRAPCON code

has been modified by changing the fuel and cladding temperature calculator from the method of weighted residuals to a more flexible finite-difference scheme. The radial "form factor" (fission rate) arrays generated by TUBRNP are used by both the temperature calculator and the fission gas release subroutines and are mapped into each routine.

The FRAPCON model for solid-solid contact conductance has been modified. As burnup proceeds, the heat conducted through solid-solid fuel pellet to cladding contact increases, and the heat conducted through gases in the gaps decreases. The contact conductance model is a modification of the Mikic-Todreas[12] model that preserves the roughness, conductivity, and pressure dependencies while providing a best-estimate for the range of contact conductance measured by Garnier and Begej. The GAPRS subroutine uses expressions for h_{solid} that are dependent on both the fuel-cladding interfacial pressure and the microscopic roughness. To provide a best-estimate prediction, the contact conductance calculated in subroutine GAPRS are multiplied by 2.9 for contact pressures greater than 5.9 MPa. In addition, the 1.8 multiplier on the roughness sum for closed gap has been eliminated.

The MATPRO model for cladding waterside corrosion and hydrogen pickup has been modified. A FORTRAN version of the integrated Electric Power Research Institute (EPRI) ("ESCORE" code) corrosion models for boiling water reactor and pressurized water reactor conditions has replaced the FRAPCON-2 model in subroutine CORROS. The new subroutine's call list is identical to that for the previous subroutine except that it requires the local value of the fast neutron flux. The new subroutine CORROS still provides separate calculations for boiling water reactor and pressurized water reactor types and returns the oxide layer in metres. In addition the hydrogen pickup fraction has been modified to be consistent with high-exposure PWR cladding data.

Mechanical models have been modified. Modifications are provided for the strength coefficient, the strain-hardening exponent, and the uniform strain to account for hydriding due to waterside corrosion. The CMLIMT subroutine equations predicting true yield strength and true strain at yield remain unchanged. True uniform strain is calculated using the proposed uniform strain model.

The MATPRO model for fuel rod axial growth has been modified. A modified equation replaces the current equation in subroutine CAGROW to bring in fast neutron fluence. The logic for handling the growth strains has been changed to include an accumulation of incremental strains. The cladding growth strains from the array of cladding nodal strains within the mechanical model have been eliminated because this model does not impact on the mechanical model predictions.

3.5.2 Solution Scheme of FRAPCON-3

FRAPCON-3 is a large and complex code that contains over 200 subroutines. The FRAPCON-3 subroutines have been grouped in packages, not all of which need to be compiled for every run. These packages are FRPCON (the main section of the code, including all of the thermal models; also includes the FRACAS-I mechanics model), FRACAS-I (the subroutines comprising the FRACAS-I mechanics model), and MATPRO (material properties package). Every execution requires the FRPCON package and the MATPRO package; the former contains the driver routine, the setup routines, and the thermal models. Using only these two packages restricts one to the FRACAS-I mechanical modelling option.

The code enters the first of four major loops in the FORTRAN coding, the time-step loop. The time-step loop encompasses virtually all of the remainder of the FRAPCON-3 code. In each execution of the time-step loop, the code solves for the thermal and mechanical equilibrium of the fuel rod at a new point along the rod power versus time history input by the user. Those subroutines within this loop are executed only once per time step.

Three additional loops exist in the code. The next loop encountered within the time-step loop is the gas-release loop. This loop is cycled until the value for calculated rod internal gas pressure (dependent on temperature, volume, and fission gas release) converges. The next inner loop in the coding is the axial node loop. For every pass through the gas release loop, the axial node loop sequences through each of the axial regions defined by the input.

The innermost loop is the gap conductance loop. This loop iterates on each axial node until thermal equilibrium in the radial direction is achieved. Thermal equilibrium is signified by a converged value for the calculated temperature drop from the fuel outer surface to the cladding inner surface.

FRAPCON-3 generates fuel rod response information as a function of fuel rod fabrication information, boundary conditions, and power history. This information is provided to the user in the form of printed output and in the form of plots (optional). The capability also exists to supply this information for steady-state initialization of the FRAPTRAN computer code. The information provided to the transient fuel rod analysis code consists of permanent burnup effects, such as cladding creepdown, fuel swelling, fuel densification, normalized radial power and burnup profiles, and fission gas inventory.

FRAPCON-3 has been designed with special features to aid the user. FRAPCON-3 has been dynamically dimensioned so that a minimum of core storage is required for any given fuel modelling process. Those parameters that are a function of the problem size are dimensioned to the exact size required by the axial and radial nodalization and the number of power-time steps. The user can set the core size based on the number of axial and radial nodes and the number of time steps.

4. CONCLUSION

In the sections above, five fuel performance computer codes are reviewed. As it is seen in the history of those codes, the code development or improvement activities are a continues process work and taking place in many organizations of many countries; for example, the series of FRAP-S, GAPCON-THERMAL series, and the FRAPCON series in the USA, and FEMAXI series in Japan.

In general, a fuel performance computer code can be considered as consisting of three parts: thermal analysis, a mechanical analysis, and a material properties component. The thermal analysis is for analysing temperature distribution from the centreline of a pellet to the coolant, FP gas release, and thermally induced deformation. The thermal analysis also includes also some mechanical models to calculate the thermally induced deformation of pellet and cladding, and the change in pellet-clad gap width. The mechanical analysis is for analysing mechanical interaction between pellet and cladding, and stress and strain of pellet and cladding. The last part, for the material properties, should include libraries for material properties of various fuel, gas, clad, and coolant materials.

The recent fuel design and improvement activities are focused on to extend burnup of fuel, and use of new materials. Thus, the most important limitation of codes is burnup validity limit. We may define three burnup regions: a low-burnup region (0-20 MWd/kgU), a medium-burnup region (20-40 MWd/kgU), and a high-burnup region (40-65 even 75 MWd/kgU).

The models, included in FRAPCON-3 and FEMAXI-V, are valid for the high-burnup region. However, FEMAXI-V includes many correlations for thermal conductivity of fuel pellet of some of which are not valid for high-burnup, even some correlations which are not a function of burnup. Therefore, the selection of a correlation should be made carefully in a simulation. FRAPCON-2 and GT2R2 codes include the models that are valid for the low and the medium burnup regions, while PIN99W includes some high-burnup models.

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