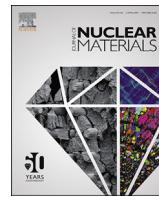




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A review of fuel performance modelling

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1. Introduction

Nuclear fuel performance modelling is performed using dedicated computer codes. Such codes exist for many fuel types and are used for a variety of purposes, including design optimization, experiment planning and interpretation, and safety analysis. In the current review, we focus on the most relevant simulation tools for the nuclear industry and disregard those that were developed only for very specific applications. As a result, we consider only codes for LWR fuel applications, since LWRs represent the dominant reactor type for civil nuclear energy production.

Nuclear fuel rod performance codes (FPCs) have been developed right from the start of the civil nuclear development programs. There have been two main categories developed, based on the conditions of operation to be simulated. These are codes simulating normal operation behavior (e.g. FRAPCON, ENIGMA, COMETHE, and FEMAXI), and codes simulating behavior in accident conditions (e.g. FRAPTRAN, TRANSURANUS, SCANAIR, TESPA-ROD, and SFPR). In recent years, there has been a tendency for both categories to develop towards each other in order to obtain tools capable of simulating fuel behavior under both normal operation and accident conditions. This was illustrated in the most recent IAEA benchmarks FUMEX-III and FUMAC.

Nuclear safety authorities, research organizations and fuel vendors in different regions of the world develop or use FPCs to predict the lifetime of a nuclear fuel rod in an LWR or a storage facility for spent LWR fuel. A list of codes is provided in Table 1; information about the historical developments, including references, can be found in Appendix: Overview of main fuel rod performance code developments across the globe (although it should be noted that there is less information provided on vendor codes, since there is less information on such codes available in the open literature).

As an invited review paper, the current document summarizes the historical developments for the fuel rod performance codes across the globe, with many references for the interested reader, rather than providing all detailed equations included in such simulation tools, for which the reader will also find appropriate references (e.g. Olander [1]) in the following sections. In view of complementary review papers being prepared for this journal in parallel, some topics will be given less attention here: fission gas behavior and the high burnup structure formation; the zircaloy cladding creep, growth and hydriding, as well as the LWR fuel failure and reliability.

We will start with reviewing the main historical developments for modelling each aspect of a fuel rod performance code, ranging from thermal, mechanical and chemical performance to neutronics modelling and microstructural changes. In the next section we review the current trends that include the applications to new fuel types as well as the implementation of advanced modelling techniques, code coupling for multi-physics applications and finally uncertainty and sensitivity analysis. In the final section of the review, we summarise the strategy for code verification and validation, along with the corresponding data, and briefly enumerate the remaining challenges.

2. Detailed advances in modelling so far

A consistent fuel rod simulation requires simultaneous consideration of the heat generation and transfer; the mechanical interaction between the fuel rod components; the isotopic evolution due to irradiation and the chemical interactions among fuel, fission products, cladding and coolant. The strong links between these aspects of fuel performance required the introduction of assumptions right from the start in order to be able obtain a sufficiently accurate numerical solution of the set of equations after a reasonable computation time. The first important assumption is about the rod geometry: most fuel performance codes still consider a cylindrical geometry and adopt axi-symmetry. In such codes, the computational domain consists of a stack of cylindrical UO_2 fuel pellets and zircaloy cladding separated by a helium-filled gap as shown in Fig. 1. The second assumption deals with the axial temperature gradient, considered to be much smaller in comparison with the radial temperature gradient. As a result, a majority of the codes (e.g. FEMAXI, FRAPCON, START and TRANSURANUS) represent the cylindrical fuel rod in a so-called one-and-a-half dimension (1.5D). In such simulation tools, all transport processes are solved in one (radial) dimension, and the axial segments are coupled via balance equations. Hence, the solution of the transport processes is usually programmed in separate modules for each axial slice, using couplers to manage interactions between models and slices. We will discuss the main features and advances made for the various aspects or parts of the codes in the next subsections.

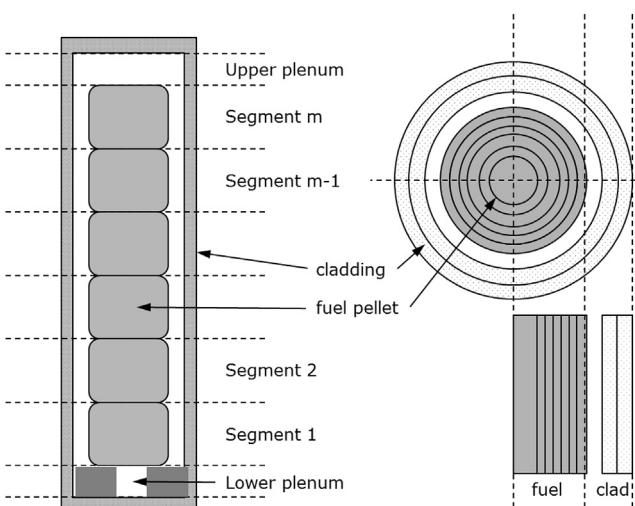
2.1. Thermal performance

The temperature distribution in a fuel rod is of primary

Table 1

List of fuel rod performance codes developed in different parts of the world for light water reactor fuel. More information is provided in Appendix: Overview of main fuel rod performance code developments across the globe.

Country	Organization	Code name (precursor codes)
Argentina	CNEA	BACO, DIONISIO
Belgium	Belgonucleaire	COMETHE
	SCK-CEN	MACROS (ASFAD)
China	Xi'an Jiaotong University	FROBA
	IAEA	FTPAC
	NPIC	FUPAC
	CGNPC	JASMINE
Czech Republic	UJV	PIN-MICRO (GAPCON-THERMAL2)
France	CEA	ALCYONE (METEOR-TRANSURANUS) Framatome COPERNIC (TRANSURANUS), GALILEO (COPERNIC/RODEX/CARO)
	EdF	CYRANO
	IRSN	SCANAIR
Germany	Siemens	CARO
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	GRS	TESPA-ROD (TESPA)
	JRC	TRANSURANUS (URANUS)
Hungary	MTA EK	FUROM (PIN-MICRO)
India	BARC	FAIR, PROFESS
	PNC	FUDA
Japan	CRIEPI	EIMUS (FEMAXI-III)
	JAEA	FEMAXI, RANNS
	SEPC	IRON (FEMAXI-III)
	NFD	TRUST
Korea	KAERI	COSMOS, INFRA
Russian Federation	VNIIM	START, RAPTA
	TRINITI	RTOP
	IBRAE	SFPR (MFPR)
Sweden	Westinghouse	STAV
	Sweden Electric	
United Kingdom	NNL, EDF Energy	ENIGMA (MINIPAT, SLEUTH, HOTROD)
USA	USNRC	FRAPCON, FRAPTRAN (FRAP), FAST
	Siemens	RODEX
	EPRI	FALCON (FREY, ESCORE)
	INL	BISON
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	Westinghouse	PAD

**Fig. 1.** Typical schematic 1.5D representation of a rod in a fuel performance code.

importance for various reasons. First of all, the conventional oxide fuels are poor heat conductors, resulting in relatively high temperatures throughout their irradiation. The fuel performance codes are therefore used for safety analyses used to ascertain that no fuel melting will occur or that the rod internal pressure will remain below a given limit. It should also be underlined that many properties and mechanisms involved in fuel rod behavior are exponentially dependent on temperature via an Arrhenius type of equation. It is therefore fair to say that an accurate temperature distribution is a prerequisite for any fuel performance code.

The heat transfer in a fuel rod in 1.5D codes is solved in a section or a slice of the fuel pin as a sequence of heat transfers between different serial heat resistances associated with the fuel, the fuel-to-cladding gap, the cladding (and its corrosion layers, CRUD, etc.) and finally the resistance between the cladding surface and the bulk of the coolant. A typical resulting temperature distribution across a pellet under normal operating conditions is shown in Fig. 2.

All thermal resistances are represented by heat transfer coefficients, except for the fuel and cladding, in which the Fourier equation is solved in cylindrical coordinates. The fission rate density or the gamma heating provide the main heat source during normal operation conditions and are dealt with in section 2.4 “Neutronics modelling” below. The other main parameter in the Fourier equation is the thermal fuel conductivity, which has been the subject of many investigations, both in pile as well as out of pile [2–9].

2.1.1. Thermal conductivity

Pioneering experimental work on the thermal conductivity of UO_2 and MOX fuel was published by Schmidt [10,11] and Gibby [2] in 1971, and a theoretical analysis was provided by Hyland [3]. Conduction of heat in the conventional oxide pellets occurs by phonons or by the kinetic energy of electrons. At temperatures below approximately 1500 K that are characteristic for normal operation conditions in LWR fuel, the phonon contribution predominates. Beyond this temperature the electronic contribution becomes important. The temperature-dependent creation of electronic carriers due to excitation of free electrons is typically expressed as [12]:

$$k_{el} = \frac{C}{T^2} e^{-\frac{W}{kT}}$$

More detailed expressions can be adopted but have only been used for specific interpretation of high temperature measurements (e.g. Ref. [13]) rather than in fuel performance codes. Theoretical considerations about atomic vibrations (phonons) lead to an expression of the phonon conductivity in the temperature range of interest. This can be expressed as

$$k_{ph} = \frac{1}{A + BT}$$

where A corresponds to the scattering of phonons by lattice imperfections such as point defects, line and planar defects, and fission gas bubbles. The parameter B corresponds to the scattering by phonon–phonon (Umklapp) interactions. This has been taken into consideration right from the start of fuel performance modelling. The effect of temperature has been measured directly out of pile by means of laser heating experiments (for example [14–20]), but also indirectly in pile by means of thermocouples inserted in the central hole of hollow fuel pellets, or in holes drilled for that purpose in a few pellets at one end of the fuel stack.

The in pile measurements are quite representative and have been applied in Risoe [21], but more extensively in the Halden Reactor Project [22]. They are indirect (i.e. they require a deeper

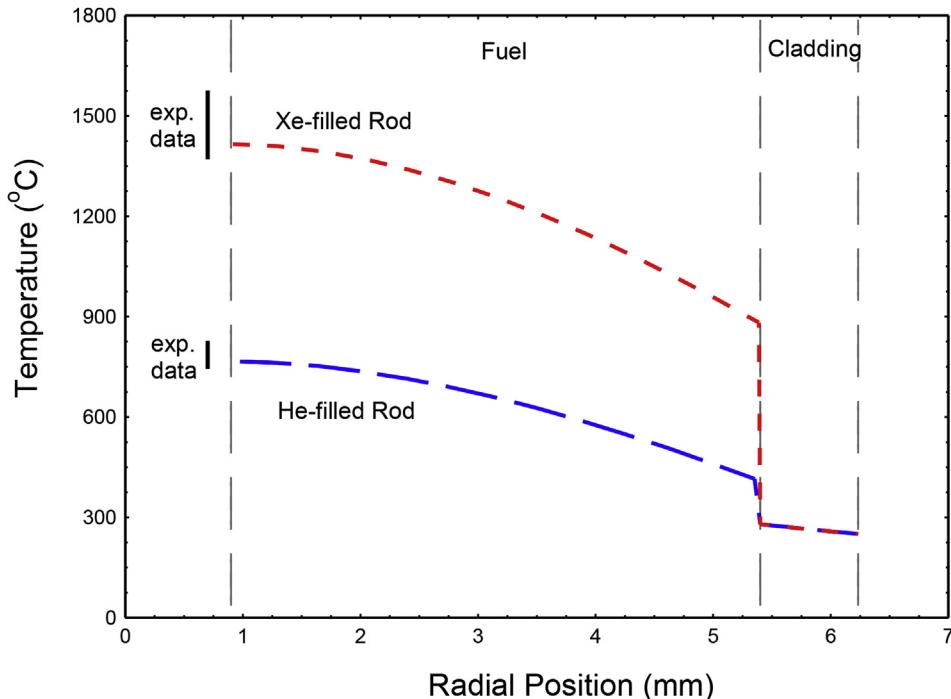


Fig. 2. Typical radial temperature distribution in a LWR fuel rod. The comparison is made between the range of experimental results obtained by means of central thermocouples and code predictions of a fuel performance code for two different fill gases (He and Xe). The experimental data from the OECD Halden Reactor Project (black, full lines) represent thermocouple measurements in the central hole of the fuel pellet, indicated by the dashed line around 1 mm.

understanding and quantification of the different phenomena that affect the central temperature during irradiation in order to infer the thermal conductivity). The vast amount of data generated and partly provided in the IPFE database, however, provided clear evidence in the 1980s for the effects of irradiation on thermal conductivity, generally referred to as thermal conductivity degradation [23]. This is attributed to the accumulation of point defects and fission products, which will increase the phonon scattering (the A term), although thermal conductivity degradation was indicated to saturate beyond approximately 50 GWd/tHM in the mid-1990s [24]. Phonon scattering can also occur when the fuel is doped with a neutron absorber such as Gd_2O_3 , or if a deviation from stoichiometry (x) occurs. In general,

$$A = A(Bu, Gd, Pu, x)$$

where Bu denotes the local burnup. Such effects have been confirmed out of pile in the 1990s thanks to laser heating experiments with both doped (e.g. Philipponneau [5] and Lucuta et al. [14–16]) and irradiated samples. The controlled temperature increase during such measurements also allowed quantification of the potential point defect annealing and resulting thermal conductivity restoration that may occur. Nevertheless, the limited impact on the central temperatures during normal operating conditions did not prompt implementation of more detailed models of thermal conductivity to be implemented in the fuel performance codes.

Another important parameter for local fuel thermal conductivity is the total amount of porosity that can impede phonon transport. It is usually homogeneously distributed in the pellets as a result of the fabrication process, but evolves over time and in space due to processes like densification or pore migration when the fuel is operated at high powers similar to those observed in fast breeder reactor fuels. Both usually occur early in life and are accounted for by means of empirical correlations or with pore migration models

subject to large uncertainties. Also, the continuous introduction of insoluble fission gas atoms can lead to the formation of additional porosity. This fission-gas-filled porosity can be in the form of very small bubbles or micron-sized pores in the so-called high-burnup structure (HBS, see “Microstructural changes”). The total porosity (P) must be taken into consideration in the local thermal conductivity, which is usually based on semi-empirical correlations that multiply the thermal conductivity expression with a correction factor depending on P , such as that proposed by Loeb [25], or more elaborated expressions derived from Maxwell-Eucken theory [26,27]. The correction factors for nuclear fuel have been discussed by Winter et al. [28] and Hayes et al. [29], whereas Bakker et al. have studied the influence of the form and orientation of porosity by means of finite element modelling [30].

In a similar way as the porosity impedes heat transfer in the pellets by interacting with the phonons, the cracks in pellets can also be thought to affect the apparent thermal conductivity of the fuel as suggested by Mac Donald et al., in 1976 [31]. One should, however, distinguish different types of cracks: macroscopic (radial, tangential and axial) cracks resulting from the thermal stresses in the fresh ceramic material as soon as the linear heat generating rate exceeds around 5 kW/m, and the microscopic cracks appearing along grain boundaries embrittled by the presence of insoluble fission gas bubbles. The latter are randomly oriented with respect to the main (radial) heat flow. Some authors suggested the effect of microcracks during transients to cause a sudden thermal conductivity degradation or temperature increase in order to explain the observed fission gas release fractions (e.g. Ref. [32]). The effect of the micro-cracks in the pellets on the fission gas release is nowadays considered directly in semi-empirical models (e.g. Refs. [33,34]). From the macroscopic cracks, only those perpendicular to the radial flow (tangential cracks) play a role. Nevertheless, their effect is now mostly embodied in the reduction of the gap size due to fragment relocation (see section 2.1.2), and can also

be justified by the relatively large uncertainty in the fuel local power (often more than 10%) [35].

2.1.2. Gap conductance

The boundary condition for the Fourier equation at the fuel center relies on symmetry, leading to a zero heat flux. At the outer surface of the fuel, a Dirichlet boundary condition usually applies, which results from the heat transfer in the fuel-cladding gap. The latter is both important and very delicate to assess as it is very sensitive to the gap size and the gas composition, hence it is strongly affected by the uncertainties pertaining to the other aspects of the fuel behavior, not the least being fuel fragment relocation at the beginning of irradiation.

The heat transfer coefficient (h_{gap}) between the outer pellet temperature ($T_{f,o}$) and the inner cladding temperature ($T_{cl,i}$) is represented by

$$T_{f,o} - T_{cl,i} = \frac{\ddot{q}}{h_{gap}}$$

and usually consists of three contributions that offer parallel thermal resistances:

$$h_{gap} = h_{rad} + h_{con} + h_{gas}$$

where h_{rad} , h_{con} and h_{gas} correspond to the thermal gap conductance due to radiation, conduction via contact points and conduction through the gas in the gap. The contribution of the radiative component typically depends on the Stefan–Boltzmann constant, the emissivity of fuel and cladding and most importantly on the fourth power of the temperature. The radiative component is usually negligible during normal operating conditions because of the limited temperatures and corresponding difference between the two opposing surfaces. During accident conditions, such as a loss of coolant accident, the temperatures in the gap become much higher and so does h_{rad} .

The component h_{con} reproduces the improvement in heat transfer due to contact pressure, for which typically an empirical term is considered rather than more elaborate models as suggested for example by Centikale et al. [36] in 1951. Simplified formulae involve the mean value (λ_m) of the thermal conductivities of fuel (λ_f) and cladding (λ_{cl}), their arithmetic mean roughness (δ_{am}) as well as the contact pressure (P_{con}) and the Meyer hardness (H) of the softer material (cladding):

$$h_{con} = C \frac{m}{\sqrt{\delta_{am}}} \left(\frac{P_{con}}{H} \right)^n$$

where C is a numerical constant, and

$$\delta_{am} = \sqrt{(\delta_f^2 + \delta_{cl}^2)}$$

represents the arithmetic mean of the surface roughness of fuel and cladding as suggested by Ross and Stoute [37]. The exponent n takes a value between 0,5 and 1 as reviewed by Herranz et al. [38] more recently.

It should be mentioned that in some cases a contribution of contact points has been considered regardless of the gap size being positive [31,39]. This is ascribed to the eccentricity of the pellet fragments after cracking, leading to some pellet-clad contact. In order to account for the resulting contact points, there are various approaches that were summarized by White [40]. Some authors define an empirical relation for the fraction of the cladding surface being in contact with pellet fragments (f_{con}), applying this as a

weighting factor for the gap conductance:

$$h_{gap} = (1 - f_{con})h_{gas} + f_{con}h_{con}$$

where f_{con} typically depends empirically on the gap size (s) and the pellet diameter (R_{pellet}), as was proposed for example by Kjaerheim et al. [41]:

$$f_{con} = c_1 + (1 - c_1)c_2^{100s/R_{pellet}}$$

Others adopted (also) a correction term for the contact pressure applied in h_{con} . More specifically, a constant value to P_{con} was added to ensure always a contact contribution. This additional term was sometimes also multiplied by a factor f_{con} .

Most models also consider a reduction in the effective gap size (s) for application in h_{gas} , which is therefore sometimes referred to as the thermal gap as opposed to the mechanical gap. The heat transfer through conduction in the gas with an average gap width is often based on the model of Ross and Stoute [37]:

$$h_{gas} = \frac{\lambda_{gas}}{\delta + s + g_f + g_{cl}}$$

where δ represents the total roughness of fuel and cladding surfaces, and λ_{gas} is taken to depend only on composition and not temperature. This is calculated by means of:

$$\lambda_{gas} = \sum_{j=1}^n \left[\frac{\lambda_j}{\left(1 + \sum_{\substack{k=1 \\ j \neq k}}^n w_{jk} \frac{c_k}{c_j} \right)} \right]$$

with c and w being molar concentrations and weighting factors, respectively. The gas extrapolation lengths g_f and g_{cl} (or temperature-jump distances) account for the imperfect heat transport across the solid-gas interface, which is material and gas-pressure dependent. Detailed formulations are suggested and discussed by Lassmann et al. [42,43].

It is important to keep in mind, however, that despite very detailed formulations for the gap conductance that were formulated in the 1960s, there is an inevitable and large uncertainty in the gap width s due to input uncertainties, as well as uncertainties in the mechanical computation (e.g. cracking, radial relocation of cracked fragments and fuel swelling). Despite this warning, it is fair to conclude that the use of central thermocouples in the Halden reactor has enabled for decades and still continues to contribute to the validation of many fuel performance codes. In particular, this verifies their ability to properly reproduce the effect of the linear heat rate, fuel rod design, fission gas release and high-burnup effects addressed above. The most recent BISON [44] and FUROM code [45] validations serve as examples (see example in section 4.3).

2.1.3. High burnup structure thermal performance

The gradual increase of the fuel discharge burnup in nuclear power reactors, and the continuous monitoring of central temperatures in experimental reactors, prompted further research on the HBS. Its effects have been incorporated in fuel performance codes as well.

First of all, the influence on the heat transfer is typically embodied directly in the thermal conductivity correlation mentioned above. It is derived from central temperature measurements like in Halden [22], in combination with thermal conductivity assessments by means of laser heating on irradiated

samples, as reviewed by Baron in 1998 [6,24]. It turned out that the overall effect of the HBS on the local thermal conductivity is more complex than that porosity evolution alone may suggest. More precisely, laser flash measurements on discs irradiated in the frame of the High Burnup Rim Project [46–49] and commercial PWR fuel in the 2000s revealed a kind of restoration when the HBS is formed [7,50]. This has been attributed to the removal of fission products and fuel restructuring in the matrix, somewhat similar to the defect annealing observed with increasing temperatures, and was also inferred from the lattice parameter evolution [24] at the end of the 1990s. Similar observations were reported by Yagnik in the frame of the NFIR project in 2000 [51]. The thermal conductivity degradation mentioned above thus tends to saturate, which prompted modelers [52] to propose at the end of the 1990s an alternative expression

$$k = \frac{\sqrt{k_0}}{D\sqrt{bu}} \tan^{-1} \left(D\sqrt{bu} \sqrt{k_0} \right) + k_{el}$$

where k_0 is given by the expression for phonon conductivity above and D is a constant.

The second impact of the HBS on thermal conductivity fuel in all performance codes is via the porosity buildup (see “Microstructural changes”). Some codes (e.g., TRANSURANUS [53]) can also consider an improved gap conductance in order to account for the bonding layer that gradually builds up between the ceramic pellets and the metallic cladding once they are in contact. For this purpose, the roughness can be empirically reduced above a certain burnup in order to simulate the filling up by mainly zirconium oxide, which has a smaller thermal resistance in comparison to the gas mixture in the residual gap. Nevertheless, the overall effect on the central temperatures is rather small.

2.2. Mechanical performance

The structural analysis of nuclear fuel rods is essential in assessing the cladding tightness for it is an important barrier against the release of radioactive products. The deformation and stresses in the fuel and cladding also impact directly the gap separating both, hence it is also strongly correlated with the thermal performance of the rod. This tight link, in turn, makes the coupling of both thermal and mechanical performance modelling challenging from a numerical point of view. In fact, the success or failure of a fuel performance code has often been determined by their convergence schemes (e.g. Refs. [54,55], for the TRANSURANUS code).

Despite its obvious interest nowadays, the mechanical performance only received sufficient attention once concerns appeared related to cladding swelling at increasing burnup levels in fast breeder reactor (FBR) fuel pins, and cladding failures in LWRs due to pellet-cladding interaction. Weeks [56] summarized the structural analysis of reactor fuel elements that started by the end of the 1960s. The SMiRT conference series played a central role, providing a platform for the developments since 1971, as reviewed by Billone et al., in 1992 [57]. Pioneering work of Gittus [58] for the theoretical analysis and by Rashid [59] and Lassmann et al. [60,61] for the code structure (for FBR fuel) are very representative for the basis of codes that are currently still used by industry (for LWR fuel). More precisely, in conventional fuel performance codes, the assessment of the stresses and strains in a section of the fuel rod is commonly based on the solution of the equilibrium relation, the compatibility equation and the constitutive equations [62]. The boundary condition at the outer surface is determined by the coolant pressure and either the rod inner gas pressure in the event of an open gap situation or the contact pressure between the fuel and the cladding

when the gap is closed. The boundary condition at the pellet center is determined by the inner gas pressure in the case of hollow pellets, and by the equality of the tangential and radial deformation in the event of solid pellets.

Many phenomena were taken into account from the start: thermo-elasticity of the fuel, thermal and fission induced creep, gaseous and solid fission product swelling, hot pressing and sintering along with migration of fabrication porosity that may result in restructuring and formation of a central hole (typical for FBR conditions), and of course pellet cracking and relocation. A detailed description of these phenomena can be found in the original book of Olander from 1976 [1]. These phenomena require material properties that account for the specific temperature, neutron flux and stress regimes.

The MATPRO handbook has been generated at the INL for this purpose [63]. It describes the materials properties correlations and computer subcodes developed for use with various LWR fuel rod behavior analytical programs. Formulations of fuel rod material properties, which are generally semi-empirical in nature, are available for conventional nuclear materials (uranium dioxide and mixed uranium-plutonium dioxide fuel, zircaloy cladding, and fill gas mixtures). The library thus contains mechanical and thermal properties applied in fuel performance codes, and was already released in the 1970s.

In 1-D fuel performance codes, the mechanical modelling must necessarily be performed at a certain elevation within the pellet. This is universally chosen to be the pellet mid-height (or pellet waist) elevation, where a plane axial strain condition applies. The complications of pellet end effects, including the impact of any dishes or chamfers, can then be ignored in the mechanical simulation. In contrast, dishes and chamfers are usually modelled explicitly in 2-D or 3-D codes via a suitable finite element mesh.

2.2.1. Fuel cracking

The cracked nature of fuel pellets complicates the mechanical analysis. There are two main approaches to modelling the effects of pellet cracks on the stresses and strains [64], both of which are only approximate. The first method models directionally dependent or anisotropic fuel elastic constants (Young's modulus and Poisson's ratio). The second method models “crack strains” (i.e., the dimensions of the cracks as fractions of the corresponding pellet dimensions) in the stress-strain relations, which relieve the stresses when the rupture stress is exceeded. As discussed below in the current trends (see section 3.2.2), with 2-D and 3-D codes there is a, potentially more accurate, third approach, which is to model the cracks, and the resultant effects on stresses and strains, explicitly. This is done by use of a suitable mesh (where a fixed number and geometry of cracks is modelled from beginning of life). More accurate again would be to model the cracking process itself (and the consequent through-life development of cracks), but, to our knowledge, this has not yet been achieved in a fuel performance code.

Radial (r - z plane), circumferential (theta- z plane) and axial (r -theta plane) cracks have all been observed in post-irradiation examination, and can all be simulated using the methods described above. However, only radial pellet cracks are usually modelled, since it is generally assumed that only such cracks propagate to a significant extent through the whole cracking plane of interest (the r - z plane in this instance). Nevertheless, circumferential and/or axial cracks are simulated in some fuel performance codes (for example, ENIGMA).

2.2.2. Small versus large strains

The conventional fuel performance codes assess the radial displacement or strain in each axial section of the rod. Strain is a

measure of deformation. In one-dimensional analyses, strain is purely in the normal direction (tensile or compressive); in multi-dimensions, strain can include shearing.

Strain is a dimensionless quantity, often defined as the ratio of one length to another. One-dimensional 'engineering' strain, on one hand, is defined as the change in length divided by the original length. 'True' or 'natural' strain on the other hand is defined as the change in length divided by the current length, whereas the 'Lagrangian' strain is defined as $\frac{1}{2}[C - I]$, where $C = F^T F$ and F is the deformation gradient:

$$F = \frac{dx}{dX} = \frac{d(u + X)}{dX} = \frac{du}{dX} + I$$

with I being the identity tensor. Expanding $F^T F$ leads to:

$$\left(\frac{du}{dX} + I\right)^T \left(\frac{du}{dX} + I\right) = \left(\frac{du}{dX}\right)^T \frac{du}{dX} + \left(\frac{du}{dX}\right)^T + \frac{du}{dX} + I$$

Whereas the engineering and true strains are linear functions of displacement, the Lagrangian strain is nonlinear due to the term:

$$\left(\frac{du}{dX}\right)^T \frac{du}{dX}$$

At small displacements, the Lagrangian strain is essentially identical to the engineering strain. In fact, at small displacements, all strain measures are equivalent.

Fig. 3 shows the differences in strain measures for the three strains defined above as well as for the Eulerian strain (a nonlinear strain measure similar to the true strain) and the logarithmic (Hencky in three dimensions) strain (defined in one dimension as the natural logarithm of the current length divided by the original length). It is clear that all give essentially the same values at small displacements.

All of these strain measures are valid models of strain. However, to capture material behavior accurately when undergoing large deformation, a nonlinear strain is needed. The rule of thumb in mechanics is that a strain larger than ~1% is large and requires a nonlinear strain measure.

The treatment of large strains in three dimensions requires managing not only large stretching but also material rotation. Recall that the deformation gradient, F , is defined as:

$$\frac{du}{dX} + I$$

This rank-two tensor can be decomposed into two tensors, $= RU$. R is an orthonormal rotation tensor that acts to rotate but not stretch a vector. U is the stretch tensor and acts to stretch, but not rotate, a vector. $F^T F$, used in the Lagrangian strain measure, is:

$$U^T R^T R U$$

Since $R^T R = I$, we have $F^T F = U^T U$. A full treatment of nonlinear three-dimensional strain is not practical here, but we note that the rotation of material implies the rotation of the stress state. This must be done in an incremental form in most cases. Rashid [65] provides a practical approach.

Whatever the strain measure chosen in an analysis, it must be used in conjunction with a constitutive law. Care must be exercised to ensure that the strain measure and constitutive law are compatible at large strains.

Strains in LWR fuel rods are generally small, and a linear representation will suffice in most cases. Since the end of the 1990s, however, there has been a tendency for fuel performance codes to be extended in order to deal with design-basis accident conditions, such as a LOCA. One of the main features in this event, from the mechanical point of view, is the appearance of clad ballooning (i.e., large strains). For that reason, some fuel performance codes have recently implemented large strain capabilities:

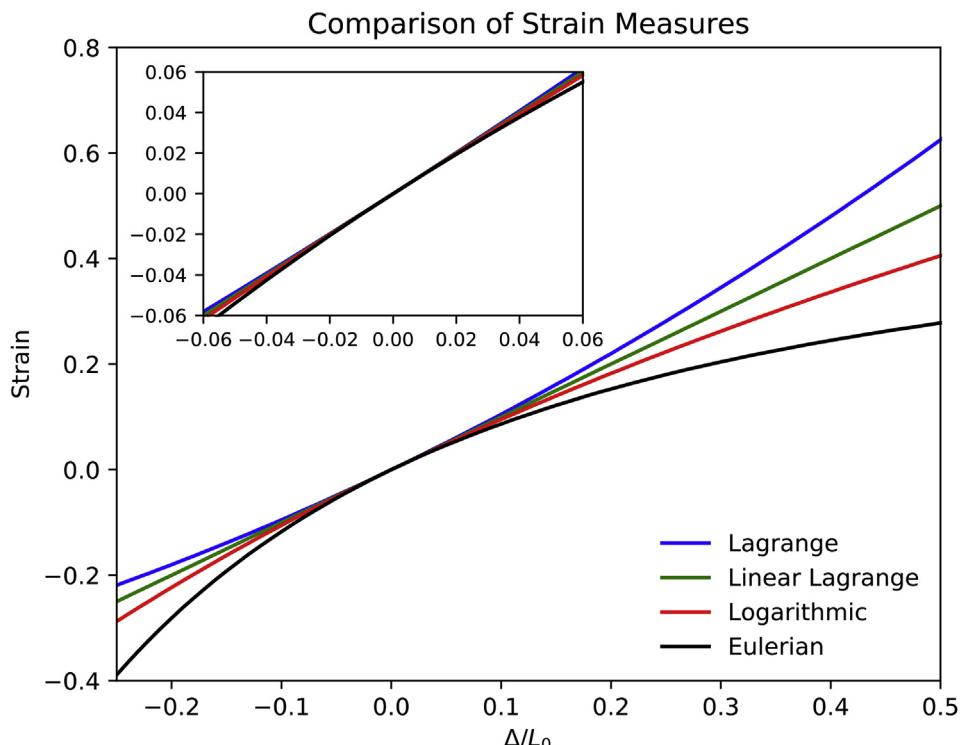


Fig. 3. Differences in strain measures for three definitions of strain defined in the text as a function of the relative displacement.

- The FRAPCON/FRAPTRAN codes [66,67] utilize a true strain measure. Furthermore, only small cladding deformations (<5% strain) are meaningfully calculated by FRAPCON-3 [66], whereas FRAPTRAN uses a special ballooning model to address material instability associated with LOCA [67].
- The FALCON code uses a small strain Lagrangian measure (dropping the $\left(\frac{du}{dx}\right)^T \frac{du}{dx}$ term) for the fuel and the complete Lagrangian measure for the cladding. Without the nonlinear strain measure in the cladding, "ballooning could not be correctly predicted" [68,69].
- The BISON code has Lagrangian small strain, Lagrangian large strain, and a full nonlinear strain measure available [70]. Similarly, Helfer [71] used logarithmic strain to extend mono-dimensional fuel performance analysis in the ALCYONE code, originally written in the framework of the infinitesimal strain theory, to cope with large deformation of the cladding during design basis accidents.
- Di Marcello et al. studied large strain in TRANSURANUS [72], which also make use of the true strain. In that work, which includes a rather complete discussion of one-dimensional strain in the context of its use in a constitutive law, it was shown that a small strain measure used in a case of large strains causes unacceptably large material volume change. Upon a switch to a large strain measure (from true strain to Eulerian), volume conservation was obtained. This work also demonstrated improved predictions on both burst tests and a loss of coolant accident (LOCA) case when using a large strain measure.

2.2.3. High burnup structure mechanical properties

As explained in more detail in Ref. [73], UO_2 undergoes an in-reactor transformation resulting in large pores and significantly smaller UO_2 grains at sufficiently high burnup below a temperature threshold. This HBS forms at the pellet periphery, where burnup can be more than double the pellet average burnup and temperatures remain relatively low. This structure is typically restricted to a few tens to hundreds of μm in width. Given the markedly different microstructure of HBS, including grains sizes of a few tenths of μm and pores ten times that size, the thermophysical properties of HBS and their effect on fuel rod performance are natural areas of investigation.

The effect of the long irradiation time on material properties applied in the equations for the mechanical performance of a nuclear fuel rod are essentially the elastic properties of the bulk materials (Young's modulus) and the amount of porosity, while the temperature changes provide an additional indirect influence (see the section entitled, "Thermal performance"). The radial variation of the hardness and fracture toughness in high burnup fuels were intensively measured by Spino et al. [74–76] by means of micro-indentation in the 1990s. More recently, Cappia et al. [77] and Terrani et al. [78] have complemented this type of analysis, whereas acoustic measurements [79–81] confirmed the trend. The results reveal that the Vickers hardness remains relatively constant across the pellet radius, except for the periphery in which the hardness is reduced up to 30% compared with the average and could be correlated with the porosity build-up of the HBS. The correlation for Young's modulus available in TRANSURANUS has been updated recently to account for burnup effects [77], and is illustrated in Fig. 4.

The original correlation components, namely the base Young's modulus, the effect of porosity, and the effect of temperature, were left intact and a new local burnup effect term was introduced. This term reduces Young's modulus with increasing burnup, although

the softened Young's modulus showed a small impact on overall simulation results.

The effect of fuel to clad bonding at high burnup is usually not considered in fuel performance codes. However, most codes deal with the effects of the high discharge burnup on cladding properties. The process of outer cladding corrosion and concomitant hydrogen uptake not only reduces the metallic clad wall thickness, it also affects the mechanical properties. The fraction of hydrogen absorbed by the zircaloy depends on the composition and heat treatment of the cladding and is usually introduced as a fitting constant. This fraction tends to concentrate in the cold part of the cladding where it can precipitate and form brittle hydrides when the concentration exceeds the solubility limit. More details about the high burnup effects on cladding are described in two specific review papers [82,83].

2.3. Chemical performance

Chemical phenomena that affect LWR fuel performance include: (a) fuel-clad bonding due to the chemical reaction between fuel pellets and cladding; (b) corrosion (oxidation) of the cladding by the coolant; (c) corrosion (oxidation) of the fuel pellets by the coolant after cladding failure; (d) changes in speciation of the fuel (including changes in the fuel stoichiometry) as irradiation proceeds (due to the depletion of fissile atoms, the generation of free oxygen and fission product atoms, and the transmutation of fissile, fertile and fission product atoms by neutron capture); (e) corrosion of the inner wall of the cladding due to reaction with the free oxygen in the rod; (f) stress-corrosion cracking (SCC) of the cladding; and (g) hydride precipitation and dissolution in the cladding (as a result of pickup, and subsequent transport, of hydrogen generated by coolant-induced cladding corrosion). Note that (d) has consequential effects on fuel swelling, actinide transport, oxygen transport and fission product transport, and (g) has consequential effects on cladding mechanical behavior, but these are not chemical phenomena themselves.

Most LWR fuel performance codes do not attempt to simulate post-failure behavior; hence, (c), corrosion of the fuel pellets by the coolant after cladding failure, is usually ignored. Of the six remaining chemical phenomena described above, the majority of currently used LWR codes only model one: (b), corrosion of the cladding by the coolant. An empirical adjustment to the fuel stoichiometry may also be made as a function of burnup (since some of the fuel thermophysical properties, as well as the fission gas atom diffusion coefficient, are strongly dependent on the fuel stoichiometry), and the mechanical effects of fuel-clad bonding (but not the bonding itself) may be simulated by activating a bonded fuel-clad contact condition (no relative motion of fuel pellets and cladding) under certain conditions (often as simple as a fixed burnup threshold). Exceptions include SFPR, ALCYONE and BISON,¹ as described below.

Via the integrated MFPR fission product release code (which itself [84] is based on the VICTORIA code [85]), SFPR models the changes in speciation of the fuel as irradiation proceeds via modules for (a) calculation of the generation, decay, transmutation and transport of over 200 fission product (FP) isotopes, and (b) calculation of partitioning of the fission product elements (considering a set of 15 fission product classes represented by Xe, Cs, I, Te, Ba, Sr, Zr, Nb, Mo, Ru, Ce, Eu, La, Nd and Sb) into phases (solid solution, grey, white, gaseous, and solid CsI) with speciation of the phases and the

¹ AMP (JNM 441 (2013) 240–251) and TRAFIC (JNM 204 (1993) 173–179) are not included here, despite them having advanced chemical modelling, since they are not, as far as we are aware, currently used for LWR applications.

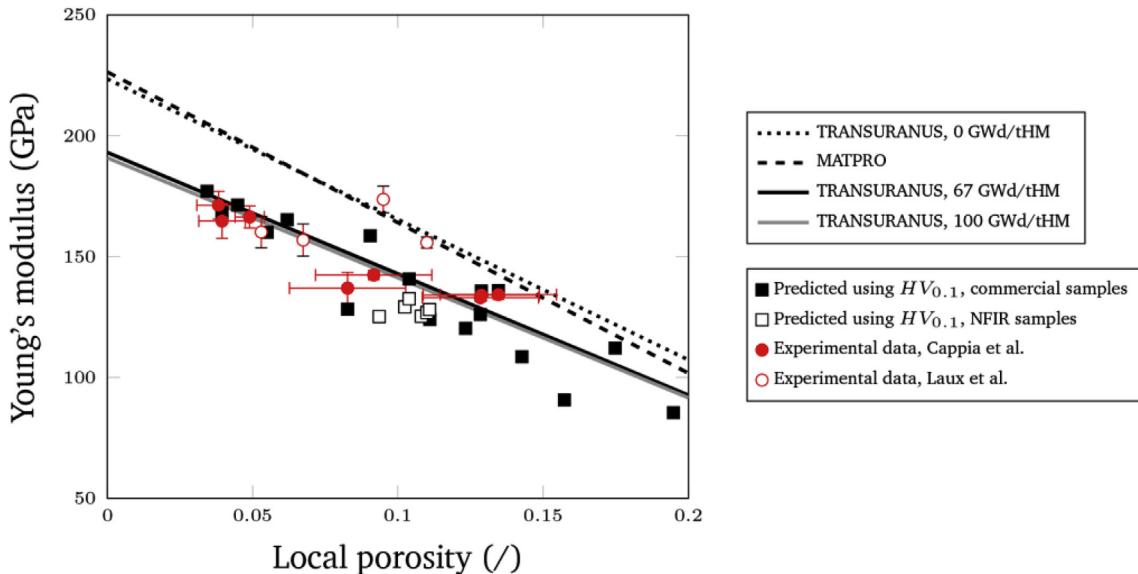


Fig. 4. Young's modulus as a function of local porosity (by Laux et al. [79] and Cappia et al. [77]), and comparison to correlations used in fuel performance codes [77].

fuel stoichiometry determined via thermodynamic equilibrium considerations for the U-FP-O system [84,86]. The oxygen potential is calculated [87] using the empirical correlations determined by Lindemer and Besmann [88] based on measurements of oxygen partial pressure and stoichiometry as a function of temperature for fresh fuel.

Via the coupled ANGE thermo-chemistry code, ALCYONE models the changes in speciation of the fuel as irradiation proceeds in a similar manner to SFPR, with the notable difference that fission product transport (limited to fission products in the gaseous phase) is computed only for xenon, with mobility assumed to be the same for other gaseous fission products [89]. Calculation of the generation, decay and transmutation of the fission product elements (considering a set of 14 fission product classes represented by Xe, Cs, I, Te, Ba, Zr, Mo, Ru, Pd, Ce, Eu, La, Gd and Pu²) is performed using correlations determined from the output of the CESAR depletion code [90]. The resulting fission product element concentrations are then used in a Gibbs free energy minimization routine to calculate the partitioning of the fission product elements into phases (solid solution, liquid, solid and gaseous) and the speciation of the phases (whether the fuel stoichiometry is also calculated is unknown), assuming thermodynamic equilibrium.

BISON models hydride precipitation and dissolution in the cladding [91,92] (although the impact of this on cladding mechanical properties is not yet simulated). The spatial distribution of hydrides as it evolves over time is calculated using models for hydrogen pickup, diffusion (using Fick's law) in the solid solution, thermo-diffusion (the Soret effect) in the solid solution, precipitation (at a rate determined by the supersaturation of hydrogen in solid solution, that is, by the excess hydrogen concentration in solid solution relative to the terminal solid solubility solvus for precipitation) and dissolution (at a rate determined by the amount by which the hydrogen concentration in solid solution is below the terminal solid solubility solvus for dissolution). The terminal solid solubility solvi for precipitation and dissolution used are those experimentally determined by McMinn et al. for unirradiated zircaloy [93] (despite different solvi for irradiated zircaloy also being

available from the same reference). The orientation of the hydride platelets (which is important for the impact on cladding mechanical properties) is not yet predicted. An example prediction of the spatial distribution of cladding hydride content is shown in Fig. 5.

The thermo-chemistry modelling capability of THERMOCHEMICA [94] (calculation of phases and their compositions for a prescribed chemical composition, temperature and pressure, assuming thermodynamic equilibrium) has been coupled to BISON to allow calculations of chemical phases, stoichiometry and oxygen potential in thermodynamic equilibrium conditions [95]. Predicted oxygen potential values for a PWR UO₂ fuel pellet irradiated to very high burnup (102 MWd/kgHM) show good agreement with measurements (obtained using a miniature solid-state galvanic cell) published by Walker et al. [96].

The fission product speciation is critically dependent on the oxygen potential, which in turn is dependent on the partial pressure of oxygen in the fuel rod. Thus, the calculation of oxygen potential using an empirical correlation (see above) represents a deficiency in the SFPR approach (as noted by Piro et al. [97]). The capabilities in ALCYONE and BISON therefore arguably set the benchmark for future modelling in this area. Such capabilities can potentially be used in the future to better understand and predict fission product speciation and transport, fuel swelling, cladding stress-corrosion cracking, cladding internal oxidation and cladding hydriding. However, the effects of radiolysis, fission-fragment-induced dissociation and hydride orientation are not currently simulated. Since these effects are important [98,99], in particular for determining the speciation of iodine and the mechanical properties of the cladding, this represents a gap in current modelling capability.

2.4. Neutronics modelling

For each timestep simulated, the power generated per unit length in each axial segment due to fission is prescribed as a boundary condition. The radially averaged power generated per unit volume in each axial segment and timestep modelled is therefore known. However, the corresponding radial profiles of the power generation per unit volume within the fuel pellets in each axial segment – which deviate significantly from uniformity as

² despite Pu not being a fission product (“fission product” is presumably used loosely to mean either a fission product or an activation product).

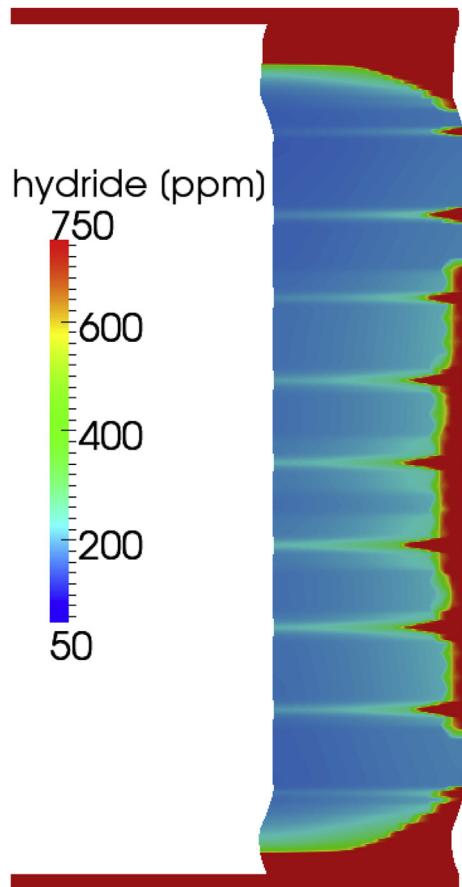


Fig. 5. Example prediction of spatial distribution of cladding hydride content by the BISON code. This is for a short rodlet containing ten fuel pellets irradiated to 65 MWd/kgHM. Note the enhanced concentration of hydrides at the pellet-pellet interfaces (radial dimension has been magnified for clarity).

irradiation proceeds, and which therefore have a significant effect on the radial temperature distributions in the fuel pellets [100] – are unknown and must be provided as input or calculated using a neutronics model. The former approach was the norm until the early 1980s, when neutronics models began to be introduced [101]. The latter approach then dominated, but the former approach is becoming more common again, in part due to the need to model advanced fuels; however, advances in computing capability mean that the provision as input now tends to be via a coupled neutronics code (see, for example, Viitanen [102]; more information is provided in “Code coupling for multi-physics simulations”).

The local power generation per unit volume at any instant depends upon the local neutron flux and its energy spectrum, the local concentrations of fissile isotopes, and the fissile isotope fission cross sections as a function of neutron energy (where “cross section” as used here and, unless otherwise noted, elsewhere in this section, means a microscopic – not macroscopic – cross section). The local concentrations of fissile isotopes in turn depend upon the prior fission, neutron capture and decay of the fissile, fertile and (if present) burnable absorber isotopes. Thus – for each timestep and axial segment – neutronics models in fuel performance codes must calculate both the radial neutron flux profile and the evolution of the radial concentration profile of the fissile, fertile and burnable absorber isotopes based on a set of fissile, fertile and burnable absorber isotope capture cross sections, absorption cross sections, fission cross sections and decay constants. The calculation of the radial neutron flux profile in turn requires a set of transport cross

sections for the isotopes in the fuel that have a significant effect on neutron transport (that is, those that have a significant effect on scattering or absorption).

The radial profiles of the concentrations of certain fission product elements arising from generation, transmutation and decay (that is, prior to any transport) are required as “source terms” for certain models: the concentrations of gaseous fission product elements – principally Xe, Kr and He – are required for fission gas swelling and release models, and the concentrations of volatile fission product elements – principally I and Cs – are required for any volatile fission product release models (which in turn can be used for activity calculations or for input to other models, like cladding stress-corrosion cracking models). Crude calculations of local fission product element concentrations can be made by multiplying the local burnup by the cumulative fission product element yield (weighted according to the yields from the different fissioning isotopes where necessary) and the local fuel density and dividing by the recoverable energy per fission. This is generally sufficient for Xe, Kr, I and Cs. However, in the case of helium this ignores the significant concentrations generated by alpha-decay of the transuranic isotopes and by the (n,α) reaction in ^{16}O [103]. Thus, several neutronics models – including RADAR [104], TUBRNP [105] and PRODHEL [106] – incorporate calculations of helium generation via these two mechanisms and ternary fission.

Other than the development of PRODHEL, the development of specific neutronics models from the early 1980s to 2010 has been summarized by Van Uffelen et al. [101]: the RADAR model from 1982 [100] (used in ENIGMA [107]) was the first significant model and was developed further to create the TUBRNP model in 1994 [108] (used in TRANSURANUS [109] and FRAPCON [110]); TUBRNP, in turn, influenced the development of RAPID in 2000 [111] (used in COSMOS [112]), PLUTON in 2001 [113] (used in FEMAXI [114] and MACROS [115]), and the RTOP model in 2002 [116]. The development of PRODHEL in 2007 (used in the French codes GALILEO [117], CYRANO [118,119] and ALCYONE [120,121]) was not considered, since at the time it was only used for helium production calculations and not for radial power profile computation [106].

We are not aware of any neutronics model development since 2010, other than the TUBRNP development in 2011 to incorporate calculations of helium generation (noted in the previous paragraph), further development of PRODHEL (see below), and the development of a neutronics model for the DIONISIO code in 2013 [122] (not described further here since DIONISIO is primarily used for PHWR applications). All models were developed for (undoped) UO_2 fuel, except PLUTON and PRODHEL, which were developed for both UO_2 and MOX fuel [106,113]. $(\text{U},\text{Gd})\text{O}_2$ -specific and MOX-specific versions of RADAR were developed in 1986 and 1990, respectively (unpublished work by Thomas and Hesketh, and Robbins, Thomas and Hesketh, respectively). These were consolidated with the original UO_2 version in 2000 in conjunction with some additional development [107]. Further RADAR development occurred in 2005 (unpublished work by Rossiter). The TUBRNP model was extended to higher burnups and to MOX fuel in 2008 [123]. Dedicated options for $(\text{U},\text{Gd})\text{O}_2$ were included in 2008 [124] and 2009 [125]. The PRODHEL model was extended to $(\text{U},\text{Gd})\text{O}_2$ in 2016 [121].

In part due to the complicated neutron capture and decay scheme for the actinide isotopes, the neutronics models just identified are necessarily simplified compared with those employed in neutronics codes. Their salient details are described below. In some cases, validation is partly or wholly done using predictions from a neutronics code. Cross sections employed may have been taken from the output of the same neutronics code, but this is still validation, rather than calibration (although less robust than validation using an independent neutronics code, a depletion

code, or measured data), given that accurate neutronics model calculations rely on the applicability of the simplified schemes in addition to the applicability of the cross sections modelled.

The original (1982) version of RADAR: (a) employed diffusion theory to calculate the radial profile of the thermal neutron flux, using constant values for the thermal scattering cross sections of ^{235}U , ^{238}U , ^{239}Pu and ^{16}O to determine the inverse diffusion length; (b) calculated concentrations of the ^{235}U and ^{239}Pu isotopes using differential equations for the local concentrations as a function of time, constant values for the thermal absorption cross sections of ^{235}U and ^{239}Pu , and a constant value for the thermal capture cross section of ^{238}U ; and (c) adjusted the local ^{239}Pu concentrations to include a component due to resonant capture of ^{238}U , using a calculated segment-average component distributed radially according to an empirical function of distance from the pellet outer radius (with the segment-average component calculated from the segment-average burnup, fixed values for the number of neutrons generated per fission and the recoverable energy per fission, and input values for the resonance escape probability and fast neutron leakage factor). It was validated using predictions from the WIMS neutronics code.

Details of the $(\text{U},\text{Gd})\text{O}_2$ (1986) version of RADAR are proprietary. The MOX (1990) version of RADAR defined an initial “effective fissile Pu concentration” as the initial ^{239}Pu concentration plus a factor F times the initial ^{241}Pu concentration, where F (which is greater than unity) takes into account the higher fission and absorption cross sections of ^{241}Pu than of ^{239}Pu . The evolution of this concentration with time was then calculated using the original RADAR approach for the ^{239}Pu concentration. The resonance escape probability and the inverse diffusion length were also treated as fitting parameters and set to prescribed functions of pellet outer radius and initial fissile Pu content. The new version was validated using predictions of the WIMS neutronics code.

The original (1994) version of TUBRNP extended the RADAR calculation of concentrations to include those of the ^{238}U , ^{240}Pu , ^{241}Pu and ^{242}Pu isotopes (although decay of ^{241}Pu was ignored). After modifying the parameters, the empirical function used to radially distribute the ^{239}Pu generated by resonant capture of ^{238}U was used to radially distribute all ^{239}Pu generated, and all ^{238}U lost, due to neutron capture of ^{238}U . The model was validated using: (1) predictions of the ORIGEN and KORIGEN depletion codes; and (2) measured radial profiles of Pu content and burnup for PWR and BWR fuel irradiated up to burnups of 64 MWd/kgHM.

Like TUBRNP, the RAPID model (2000) extended the RADAR calculation of concentrations to include those of the ^{238}U , ^{240}Pu , ^{241}Pu and ^{242}Pu isotopes (with decay of ^{241}Pu simulated). However, unlike RADAR and TUBRNP, local one-group neutron fluxes are defined as a function of enrichment, burnup and power generated per unit volume, with no neutron diffusion calculation, and no radial dependence assumed. Fission and capture are then modelled using these fluxes, the concentrations of the various isotopes, and one-group cross sections which are a function of enrichment, radius and burnup; resonant capture effects are included in the capture cross section of ^{238}U . The model was validated using: (1) predictions of the HELIOS neutronics code; and (2) measured radial profiles of Pu content and burnup for PWR and BWR fuel irradiated up to burnups of 70 MWd/kgHM.

The 2000 version of the RADAR model extended the calculation of concentrations to include those of the ^{238}U , ^{239}Np , ^{240}Pu , ^{241}Pu , ^{241}Am and ^{242}Cm isotopes (with decay of all isotopes simulated). The calculation of ^{241}Am and ^{242}Cm concentrations was to allow the generation of helium via ^{242}Cm alpha decay to be evaluated; helium generation via ternary fission was also computed. Resonant capture was modelled using dedicated resonant capture cross sections in both ^{238}U and ^{240}Pu , and scattering cross sections were replaced by

transport cross sections in the calculation of the inverse diffusion length. All cross sections for UO_2 were made a function of enrichment, and all cross sections for MOX were made a function of plutonium content. The new version was validated using predictions of the CASMO-4 neutronics code.

Like TUBRNP, the PLUTON model (2001) calculates the concentrations of the ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu and ^{242}Pu isotopes. Unlike TUBRNP, a three-group scheme is followed, with neutron fluxes and cross sections calculated separately for neutrons in thermal, resonance and fast energy groups. In addition, the resonant absorption cross sections are computed via the calculation of resonance integrals based on theoretical considerations. The model was validated using: (1) predictions of the ORIGEN and KORIGEN depletion codes; and (2) measured radial profiles of Pu content and burnup for PWR and BWR fuel irradiated up to burnups of 70 MWd/kgHM.

The RTOP model (2002) follows a similar scheme to PLUTON, but in two – thermal and superthermal – energy groups. The concentration of the ^{236}U isotope is also calculated. The superthermal flux is computed from the thermal flux using a defined ‘spectrum hardness parameter’. The model was validated using: (1) predictions of the KORIGEN depletion code; (2) measured radial profiles of Pu content and burnup for PWR and BWR fuel irradiated up to burnups of 83 MWd/kgHM; and (3) measured concentrations of the U and Pu isotopes in VVER fuel irradiated to ~30 MWd/kgHM.

In order to better calculate helium generation, the 2005 version of the RADAR model extended the calculation of concentrations to the ^{238}Pu and ^{242}Am isotopes (with the calculation of the concentration of ^{239}Np omitted) and extended the calculation of helium generation to that from the (n,α) reaction in ^{16}O . Like RTOP, the neutron flux and cross sections are computed in thermal and superthermal energy groups. Cross sections are dependent on enrichment (UO_2), gadolinia content ($(\text{U},\text{Gd})\text{O}_2$), plutonium content (MOX), pellet outer radius, burnup, and/or distance from the pellet outer radius, as appropriate. The updated version was validated using predictions of the CASMO-4 neutronics code.

The 2007 version of the PRODHEL model calculates the concentrations of 22 actinide isotopes from ^{235}U to ^{244}Cm (with decay of all isotopes simulated) in order to calculate the radial power profile and helium generation from alpha-decay. Helium generation due to ternary fission and the (n,α) reaction in ^{16}O is also calculated. Burnup-dependent one-group cross sections are employed. Of note is that $(\text{n},2\text{n})$ reactions are considered, for which those in ^{238}U and ^{239}Pu are relevant for production of ^{238}Pu (via beta-decay of ^{237}U , neutron capture of ^{237}Np and beta-decay of ^{238}Np in the case of the former). The code was validated using: (1) predictions of the APOLLO2 and CESAR neutronics codes; and (2) measurements of actinide isotope concentrations obtained from chemical analyses of spent LWR fuel.

The 2008 version of the TUBRNP model extended the calculation of concentrations to the ^{236}U , ^{237}Np and ^{238}Pu isotopes. The calculation of the ^{238}Pu concentration included use of a “recursive analytical algorithm” to determine the contribution from ^{242}Cm alpha decay (without explicit calculation of the concentration of ^{242}Cm). Updated one-group cross sections for UO_2 and MOX were also introduced, including ^{238}U and ^{240}Pu capture cross sections with a strong radial dependence to take account of resonant capture effects. The model was validated using: (1) predictions of the ALEPH neutronics code; and (2) measured radial profiles of Pu content and burnup for LWR and VVER UO_2 fuel irradiated up to burnups of 102 MWd/kgHM, and for LWR MOX fuel irradiated up to burnups of 45 MWd/kgHM.

In order to simulate Gd-doped fuels, the TUBRNP model has since 2008 applied effective cross sections for total and for thermal neutron absorption of ^{155}Gd and ^{157}Gd [124]. The model was

validated (1) against radial profiles of local power density and local Gd concentrations predicted by the HELIOS code for $(U,Gd)O_2$ fuels with an initial gadolinia content of 2.0 wt% and 8.0 wt% and (2) indirectly against in pile measurements of fuel center temperatures performed at the Halden BWR for $(U,Gd)O_2$ with the above mentioned gadolinia contents. A specific extension of TUBRNP for Gd-doped VVER fuels was introduced in 2009 [125]. It applies burnup-dependent radial form factors accounting for the resonant capture of neutrons in ^{155}Gd and ^{157}Gd and was validated against predictions by Monteburns (a coupling of MCNP and ORIGEN).

The 2011 version of the TUBRNP model includes the calculation of helium generation. The helium generation contribution from alpha-decay is determined from the concentrations of the isotopes already calculated, together with new calculations of the concentrations of ^{241}Am , ^{243}Am , ^{242}Cm and ^{244}Cm . Contributions from ternary fission and the (n, alpha) reaction in ^{16}O are also computed. The model was validated using: (1) predictions of the VESTA neutronics code; (2) measured radial profiles of Pu content and burnup as per the 2008 version validation, but including some additional 81 MWd/kgHM LWR UO_2 data; and (3) measured concentrations of U, Pu, Am and Cm isotopes as a function of burnup from the NEA's SFCOMPO spent fuel isotopes database.

The 2016 version of the PRODHEL model extended the 2007 version to $(U,Gd)O_2$ by adding calculations of the concentrations of the ^{155}Gd and ^{157}Gd isotopes. Two-group cross sections are used, as opposed to the one-group cross sections used in the earlier version. The updated version was validated using predictions of the APOLLO2 neutronics code.

In conclusion, variants of the RADAR, TUBRNP and PRODHEL neutronics models are the main ones in use today for LWR applications. Modelling has converged towards combined calculation of radial power profile and helium generation for UO_2 , $(U,Gd)O_2$ and MOX fuel via calculations of the concentrations of the actinide isotopes. There are some differences, including: (a) the isotopes, reactions and number of neutron energy groups considered; (b) the dependencies of the various cross sections on fuel characteristics (enrichment, pellet outer radius, etc.) and burnup; and (c) the nature and extent of the validation. Recent development of neutronics models is limited, in part because increases in computing power allow, and applications to new fuel types require, coupling neutronics codes to fuel performance codes rather than using neutronics models.

2.5. Microstructural changes

2.5.1. Grain growth

First of all, we should point out that we limit ourselves to normal or equiaxed grain growth [126], because columnar grain growth is associated with bubble migration by means of evaporation and condensation, which is typical for fast reactor conditions (at temperatures above approximately 2000K).

The driving force for grain growth is the reduction of the free energy of the solid that accompanies the decrease of the area of the grain boundaries it contains. During normal grain growth, large grains grow at the expense of smaller ones and therefore affects the fission product release in two ways [73]. On one hand, the sweeping boundary collects insoluble fission products; hence, it provides an additional mechanism for transport of fission products from within the grains by diffusion to the grain boundaries from which they can be released. The moving grain boundary thus acts as fission gas filter. On the other hand, the diffusion distance for the fission products created in the grains increases, which tends to postpone or reduce the release kinetics.

The models for grain growth in nuclear fuels are prone to large uncertainties. In general, the kinetics of grain growth are written in

the form of a simple equation $R_{\text{gr}}^n = R_{\text{gr},0}^n + Kt$, where $R_{\text{gr},0}^n$ and R_{gr}^n stand for the initial and current grain size, n is the growth exponent varying between two and four, and K corresponds to a rate constant which usually has an Arrhenius form. The uncertainties are caused by the many parameters that can affect grain growth: temperature, the grain radius itself, and of course the variety of impurities in the lattice that can interact with a moving grain boundary, which include pores and second-phase particles and fission products. The latter can introduce a back stress on the moving boundary, referred to as the Zener effect. In order to cope with such parameters, the grain growth equation includes a limiting grain size (R_{max}) that can be depending on burnup as proposed by Ainscough et al., in 1973 [127]:

$$\frac{dR_{\text{gr}}}{dt} = K \left(\frac{1}{R_{\text{gr}}} - \frac{1}{R_{\text{max}}} \right)$$

For different MOX fuel compositions, grain growth measurements were reported in 1986 by Sari et al. [128], in 1990 by Bainbridge et al. [129], in 2000 by Duriez et al. [130], and in 2013 by Van Uffelen et al. [131]. Various similar empirical correlations are currently applied in the codes: for instance for UO_2 in the FEMAXI code [132] although other models reported in the literature can be selected [114], in the FRAPCON 3.5 code [66] a grain growth model proposed by Khoruzhii et al. is used [133], and in the TRANSURANUS code also different models are available. Examples include [127] for UO_2 , and more recently [131], for MOX fuel. The measurements, even on fresh fuel, still reveal a large uncertainty of about one order of magnitude on the kinetic coefficient [131].

2.5.2. Porosity development

The fabrication process of the oxide fuels applied in commercial nuclear power plants typically leaves an average porosity of about 5% in volume [35]. The pores can have a monomodal (typical radius of 4–5 μm) or a bimodal size distribution (larger second peak with radius around 10–25 μm), depending on whether a volatile pore former is used in the fabrication process [134].

A fraction of this porosity is connected to the free volume in the fuel rod and is termed open porosity. Because of its importance for so-called athermal fission gas release, several attempts were made to account for it. The most simple attempts introduced an additional empirical release term as a function of the initial open porosity fraction in the 1980s and 1990s [118,135–137]. Others (e.g. Ref. [138]) have adopted an empirical reduction of the effective sphere radius of the Booth sphere for diffusional release from the grains. In 2012, Feng et al. [139] extended this with an additional fitting parameter in the intragranular diffusion coefficient, and applied the total fabrication porosity rather than only the open porosity fraction. At the same time, Millet et al. [140,141] explored a mechanistic description based on percolation along grain boundaries, which however cannot be implemented in conventional fuel performance codes although it appears to be intuitively more appropriate when considering open porosity. Instead, it was felt that a semi-empirical model considering the porosity as a mean-field should be developed in order to use a percolation model. For this reason, in 2015 a new model was proposed [142], considering open porosity in a mechanistic manner. The new approach relies on the model for open porosity in the sintering process of crystalline solids based on the pioneering work of Coble [143] for modelling sintering in 1961 and Wong et al. [144] in 1979. In similar way as White and Tucker [145] did for their fission gas release model in 1983 and later also Koo et al. [146], the grain is represented by a tetrakaidecahedron while the open porosity is represented as a continuous cylinder along the grain edges.

Freshley et al. [134] pointed out in 1976 that at the beginning of

irradiation, typically until a burnup of 2–3 MWd/kgHM, a fraction of the total porosity (typically pores smaller than 1 μm) will disappear because of the so-called densification process, which is similar to in pile sintering under the influence of the interaction of the pores with energetic fission fragments, in a similar way as irradiation induced resolution of fission gas filled bubbles [73]. According to Freshley et al. [134], density increases occurring during out-of-reactor isothermal resintering tests are correlated with in-reactor density changes. Thus, Maier et al. outlined in 1988 that relatively simple resintering tests can be used to predict the amount of in-reactor densification that can be expected to occur for a particular fuel type [147]. Such data (e.g. final density obtained) can be provided on input to fuel performance codes for the empirical densification models applied (e.g. in, ENIGMA [148]), whereas Stehle et al. [149] suggested detailed models accounting for the grain size, temperature, fission rate density, etc, in a similar way to that for fission gas behavior models [73]. More recently, Tarasov et al. have reviewed mechanistic models for the porosity evolution in the MFPR code [150].

As the irradiation proceeds further, the fuel density evolves with the solid fission product swelling and gaseous swelling if the temperatures are high enough to promote insoluble fission gas precipitation [35]. Experimental information about UO_2 swelling is typically based on fuel stack elongation measurements in the Halden reactor during standby when there is no mechanical interaction with the cladding [151]. The measurements include the effects of densification, matrix swelling due to solute fission products and gaseous swelling due to bubble and tunnel formation; hence, they should be considered carefully. The general outcome considered in fuel performance codes is a linear inexorable volumetric swelling of around 0.7–1% per MWd/kgHM [62], which has been simulated more recently by means of molecular dynamics calculations [152].

Beyond an average burnup of about 55 MWd/kgHM, however, the formation of the HBS initiates [73] and is accompanied by an

acceleration of swelling due to formation of micron-sized porosity [74,153], starting in the self-shielded periphery of UO_2 pellets. The combined effects of densification, swelling, and HBS formation on the fuel relative density versus burnup is illustrated in Fig. 6, based on different measurement techniques such as immersion density measurements and acoustic microscopy [154].

As explained in the review of fission gas behavior [73], UO_2 undergoes a transformation in reactor resulting in large pores and significantly smaller UO_2 grains at sufficiently high burnup below a temperature threshold. This HBS forms at the pellet periphery, where burnup can be more than double the pellet average burnup and temperatures remain relatively low. It is restricted to a few tens to hundreds of μm in width. Given the markedly different microstructure of HBS, including grains sizes of a few tenths of μm and pores ten times that size, the thermophysical properties of HBS and their effect on fuel rod performance are natural areas of investigation.

Models to describe the HBS initiation and formation process have been developed since the mid-1990s in parallel to the HBRP project [46–49], and later also the NFIR project [155], for determining conditions for nucleation in terms of burnup threshold, temperature, grain size, etc. and the potential implications for design basis accidents. Such models a normally not included in fuel performance codes, and despite the numerous research efforts, there is still no consensus about the formation mechanisms and their sequence, as revealed in the review in 2010 by Rondinella and Wiss [156].

2.5.3. High-burnup structure modelling in fuel performance codes

For fuel performance codes, there have been various approaches to address phenomena associated with the HBS formation such as the porosity build up and fission gas behavior, thermal conductivity degradation and recovery, as well as the mechanical properties. The vast majority initially considered empirical correlations and model parameters. Much of the other specific HBS developments

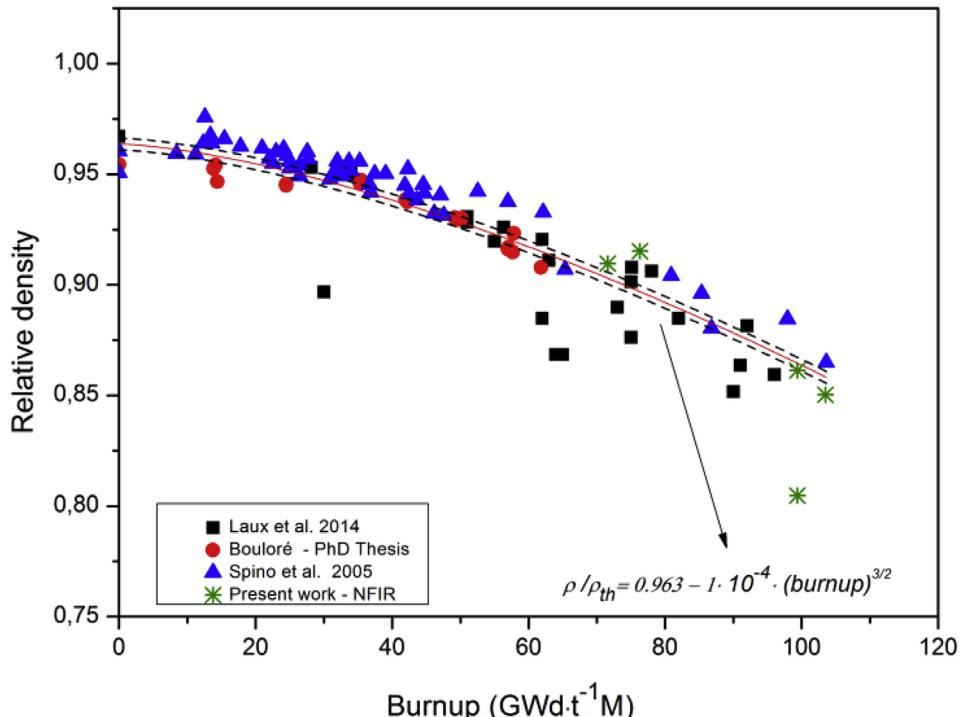


Fig. 6. Evolution of the bulk density-theoretical density ratio of uranium dioxide fuel as a function of burnup according to Ref. [154].

incorporated in the fuel performance codes have been summarized in the IAEA document published in 2012 as a result of the FUMEX-II benchmark that was dedicated to modelling at extended burnup [157]. In most cases, the codes account for the thermal conductivity degradation and porosity buildup in the fuel (e.g. BACO, CARO, COPERNIC3, COSMOS, INFRA, etc.), and very few account for an additional fission gas release associated with the HBS during normal operation (e.g. START-3 [158,159] and CARO [160]). In the FRAPCON code [66,161,162], the model of the HBS thickness, based on the size of the high-burnup rim measured by optical microscopy [163], has been used since the mid-1990s. The porosity in HBS was also modelled based on a fit to observations on high burnup fuel [74,164,165].

In 2000, Suzuki et al. [166] introduced models in the FEMAXI-V code for (a) the volumetric ratio of the HBS formation, (b) the amount of gas retained in the matrix and in the corresponding HBS pores, (c) the amount of swelling caused by the HBS, and (d) the effect of the HBS porosity on the thermal conductivity. The models can be selected via input options.

In parallel in Korea, Lee et al. [111,167] developed the INFRA (INtegrated Fuel Rod Analysis) version for predicting the fuel rod behavior at high burnup. Apart from the RAPID model [111] for the radial power profile, various new models that can predict a high-burnup effect up to a 70 MWd/kgU were also developed [168]: (1) an empirical model for the rim structure formation as function of temperature and local burnup, inferred from a more detailed scenario [169]; (2) irradiated fuel thermal conductivity; (3) fission gas release. Part of the validation for the INFRA code was reported in the FUMEX-II benchmark organized by the IAEA [157,170]. The COSMOS code does not contain a specific modelling of the HBS structure, but implemented the usual thermal correlations for thermal conductivity and radial power profiles at high burnup.

An early effort to model HBS was undertaken in TRANSURANUS [108,171] in the early 1990s based on EPMA measurements from different sources. More precisely, a model was developed to predict a linear increase in local porosity up to a certain limit, to track intragranular Xe in HBS as well as the thickness of the transition zone between typical UO₂ and of the HBS itself. It relies on the concept of a threshold burnup beyond which the fission gas is removed from the matrix to form pores according to a rate that is proportional to the gas concentration. This concept was later extended by Holt et al. [172] because the scatter in local threshold burn-up values for HBS formation is expected to be affected by the local temperature [173]. This is because defect annealing is assumed to impede HBS formation; this was also considered in the empirical approach presented by Sontheimer et al., in 2000 [174], as well as in the COPERNIC3 code for the HBS porosity development [175]. In line with this idea, Khvostov et al. developed a model in the beginning of the 2000s [158,159,176] in the START-3 code for describing both the formation, development, and behavior (fission gas release and swelling) of the HBS in a fuel performance code as a function of the so-called “effective burn-up”. Khvostov documents a model of polygonization of the fuel grains, which informed fission gas release and porosity changes in the code. According to the model, increased porosity in the rim region also decreases thermal conductivity and increases swelling. While acknowledging the difficulty of quantifying the effect of HBS on the mechanical behavior of fuel rods, Khvostov reports improved cladding diameter comparisons when using the HBS-enhanced swelling model. His model was implemented in the FALCON code [176,177] in 2009, where the effective burnup was defined as a temperature-dependent burnup value, considering that no further accumulation of defects could contribute to the HBS formation when the local temperature exceeds a given threshold. As a result, there could be no additional increase in the effective local burnup value

used in a HBS model beyond a certain temperature. Nevertheless, the predicted upper threshold temperature of 800 °C conflicts with the experimental temperature threshold of Kinoshita et al. [46], which could be overcome by the model of Holt [172] based on a multi-physics simulation and additional EPMA data from HBRP discs, leading to a threshold temperature of about 1050 °C.

More recently, and in line with the ideas of Khvostov et al., a semi-empirical model to describe the formation of the HBS was proposed [178] for TRANSURANUS, in which the grain size reduction and the depletion of intra-granular fission gas in the crystal grain in UO₂ pellet can be treated simultaneously.

Developments for the HBS in the DIONISIO code [179] were made more recently following FUMEX-III. Recognizing that the mechanisms governing the HBS transformation have not yet been fully elucidated, some empirical expressions have been formulated to describe the behavior and progress of porosity at local burnup values ranging from 60 to 300 MWd/kgHM. The model includes the growth of the pore radius by capturing vacancies, the interactions of different orders between pores and the resulting evolution of porosity (pore number density and overpressure within the closed pores), as well as the evolution of the inventory of fission gas both dissolved in the matrix and retained in pores.

Probably the most detailed model for the development of the HBS applied in a fuel performance code today is that incorporated in the SFPR code [86]. It is currently based on the stand-alone MFPR model developed by Veschchunov and co-workers [87] in collaboration between IBRAE and IRSN. It contains a detailed set of equations for both point defects (including fission products) as well as for extended defects such as dislocations, bubbles and pores. A modified version is under development at IRSN [180]. As part of this effort, coupling and benchmarking with the TRANSURANUS code and experimental data [181] are being completed.

3. Current trends

3.1. Application to new fuel types

3.1.1. MOX fuel

Nuclear fuel rods with mixed oxide (MOX) pellets have been irradiated since the 1960s, in both LWRs as well as fast breeder reactors. MOX fuel pellets contain a mixture of uranium and plutonium oxide, enabling recycling of large quantities of fissile isotopes produced and remaining in spent UO₂ fuel. Producing MOX fuel can thus be considered as a means to utilize natural uranium resources more efficiently, although it has always been recognized that recycled plutonium would be most effectively and efficiently utilized in FBRs. Nevertheless, in the 1950s it was already generally accepted that available reprocessing capacity would exceed the requirements of the FBR prototypes planned at that time. For this reason and in order to address the feared or anticipated scarce supply of uranium at moderate prices, programs for using MOX at an industrial scale in LWRs were developed in the 1970's.

Although uranium prices have remained moderate, MOX is used in nuclear power reactors in several countries. In the US, although plutonium recycling studies began in 1956, and reached a commercial demonstration stage by 1975, all research on MOX fuel stopped in 1980 following President Carter's executive order on non-proliferation in 1977. The last MOX assemblies irradiated in U. S. plants were irradiated in the Ginna reactor and discharged in 1985.

In Europe, the world's first LWR MOX was loaded in the BR3 in Belgium, followed by the MOX loading in the VAK in 1966. In the 1960s, with increasing interest in plutonium recycling, a number of other European countries embarked on MOX utilization in LWRs.

For example France, Switzerland, France, the UK, Italy, the Netherlands and Sweden began work in this area, albeit to different extents [182].

In Japan plutonium research concentrated first on FBR fuel and fuel for the Advanced Thermal Reactor (ATR), whereas MOX use in LWRs was launched in the 1980s. For this purpose, various irradiation tests have been carried out in the ATR and transient tests in the Halden Reactor.

The design of MOX fuel is largely based on conventional UO_2 designs, with only two minor modifications. The first deals with the neutronics. In order to ensure that assemblies are (almost) equivalent to those containing UO_2 in terms of dissipated power, total reactivity, and accumulated burnup, the assemblies have been optimized to reduce power peaking at the interface between UO_2 and MOX. The lowest possible shape factor is achieved by zoning the assembly using three different enrichments in a concentric distribution in the case of PWRs and up to seven in the case of BWRs [182]. The second design change deals with the increased plenum volume, which is sometimes applied to accommodate the high fission gas release expected for MOX fuel. Indeed, due to the neutronic properties of the Pu isotopes in MOX fuel, the reactivity decreases less rapidly with burnup than in UO_2 fuel. Because of this MOX fuel dissipates more power later in life, which in turn leads to higher fission gas release. This is also affected by the lower thermal conductivity of MOX fuel, giving rise to higher fuel temperatures.

Since MOX fuels have been used in the nuclear industry for many decades, the models of MOX have been integrated into most existing fuel performance codes. As outlined above, the fuel properties and in pile performance differences between MOX and UO_2 fuel include fuel reactivity, thermal properties, and release of fission gas and helium. Efforts have been made to establish unified models adapted to both MOX and UO_2 by considering specific models for radial power profiles, with the Pu content as a factor for thermal conductivity, or by using different coefficients for MOX and UO_2 [6,9,104,105,109,183–188].

3.1.2. Doped fuel

Additives have been studied since the 1960s (e.g. Ref. [189]) with the intention of improving the sintering process and the resulting microstructure and pore-size distribution, which in turn has enabled better control of in pile densification. Driven by economic factors, the nuclear industry has continuously striven to reduce fuel cycle costs, enhance flexibility and improve the reliability of operation. This can obviously be achieved by reducing the consequences of fuel failures, but also by increasing the fuel weight and optimizing rod internal properties affecting operational margins. Several types of dopants have therefore been added to conventional UO_2 fuel in order to improve different aspects of fuel performance.

Mostly gadolinia (Gd_2O_3), but sometimes also erbia (Er_2O_3) or zirconium diboride (ZrB_2) are currently used as a burnable absorbers in high-enriched fuel rods, which in turn enables an increase in discharge burnup [190]. Both gadolinia and erbia are mixed directly with the uranium dioxide fuel; hence, they affect essentially thermal properties [12,190]. However, the effects of gadolinia on fuel performance were considered in thermal conductivity [6,191–193], radial power [125], and fission gas diffusion and release models. For example, in COPERNIC and TRANSURANUS, the ratio of $\text{UO}_2\text{--Gd}_2\text{O}_3$ thermal conductivity to UO_2 thermal conductivity is dependent on temperature and gadolinia content [193], while in FRAPCON/FRAPTRAN, the gadolinia content is considered to be a factor in thermal conductivity expression. Fission gas diffusion coefficient decreases with increasing quantities of gadolinium [44,194]. This effect is also taken in account indirectly by replacing the local temperature with a modified

temperature that depends on the gadolinium weight fraction [193]. The gadolinium content also produces a distorted, rapidly changing radial power profile [125,183,186,195]. Specific radial power tables are sometimes used for $\text{UO}_2\text{--Gd}_2\text{O}_3$ fuel [193]. The TUBRNP model for the radial power profile in the TRANSURANUS code has been extended to include the total effective neutron absorption cross section of ^{155}Gd and ^{157}Gd , either as analytical functions or as tabulated datasets [125]. This model is also used in FRAPCON to obtain radial power profile after high cross section Gd isotopes have burned out [194]. More recently, however, coupling was developed between the fuel performance code TRANSURANUS and the Monte Carlo reactor physics code Serpent [196]. The main motivation was to replace the internal diffusion approximation based neutronics solver of TUBRNP with a higher-fidelity code to improve accuracy, especially in situations where steep gradients in the neutron flux can affect the capability of the diffusion solver to yield accurate results. This can be the case, for example, in the presence of burnable absorbers such as Gd or when the fuel is located in the vicinity of a control rod.

The use of zirconium diboride in the Westinghouse-designed Integral Fuel Burnable Absorber is in the form of a thin coating of ZrB_2 on the uranium dioxide pellets. This burnable absorber works through the (n,α) reaction on ^{10}B . The modelling thereof is thus largely focused on the neutronics and the effect of the helium generation on the internal gas pressure, as was introduced in the TRANSURANUS code in 2000 [197] and more recently also the FRAPCON4.0 code [198].

Additives such as magnesia (MgO), titania (TiO_2), niobia (Nb_2O_5) and chromia (Cr_2O_3) have been shown to produce large-grained material in order to reduce fission product release, and at the same time improve the pellet-cladding interaction resistance (e.g. Refs. [199,200]). This requires the appropriate concentration of crystal growth activators together with the proper sintering conditions (oxygen potential and temperature) in order to obtain the extended grain size and intragranular precipitates that promote nucleation of bubbles and the resulting trapping of gas atoms. Other types of additives are used to modify the grain boundary characteristics: Al and Si with limited solubility are added to form a glassy phase along the grain boundaries in order to promote sintering and grain growth. As a result of the various studies with additives, BNFL has developed niobia-doped fuel [201], Westinghouse has developed ADOPT (Advanced Doped Pellet Technology) UO_2 fuel containing additions of chromium and aluminium oxides [202], Framatome has developed and tested Cr-doped UO_2 fuels [203], and TVEL and VNIINM have also implemented aluminium silicates in VVERs [204], while similar studies were carried out in China [205] and Korea [206].

In 2014 Massih reviewed the effects of the additives on UO_2 behavior [207]. He confirmed that, apart from considering larger grain sizes, the differences of the remaining physical properties of the pellets (including heat capacity, thermal expansion coefficient, melting temperature, and thermal diffusivity) between the doped and standard UO_2 pellets are small. The only exception is the increased creep rate (e.g. Ref. [208]).

3.1.3. (E)ATF

The goals of enhanced accident tolerant fuel (EATF) are to increase coping time and to mitigate the radioactive consequence under design basis or beyond design basis accidents for water cooled reactors. The desired attributes of potential EATF fuel systems include reduced oxidation compared with zircaloy cladding, improved dimensional stability and fission product retention capability [209]. Various fuel and cladding candidates have been proposed and investigated [210].

Fuel performance models, together with reactor core codes and

system codes, have been developed to reflect the development of EATF and served as a quantitative tool to assess the benefits that can be gained from various EATF candidates. For the modelling work of ATF fuel and cladding candidates, two different modelling approaches were used. Existing fuel performance codes like FRAPCON [211,212], FUPAC [213], FALCON [214], and TRANSURANUS [215] were used for simulations of USi, UN, FeCrAl, and (homogenized) SiC composite cladding with modified material properties and irradiation behaviors models. For candidates with more complex geometries, FEM codes like BISON [214,216,217], COMSOL [218–220], ADINA [221–223] and ABAQUS [214] have been used to describe the microstructure of TRISO particles in FCM fuel, laminated structure of SiC composite cladding and Cr coated zircaloy cladding.

Confidence in predictive results depends on the technical readiness level of the specific concept and detailed knowledge of the material properties, which are under continuous progress, for example in the frame of the IAEA co-ordinated research project on “Analysis of Options and Experimental Examination of Fuels for Water Cooled Reactors with Increased Accident Tolerance” (ACTOF), which was launched in 2015 for four years [224,225]. It deals with the acquisition of data through experiments on new fuel types and cladding materials, the development of modelling capacity to predict the behavior of the components and the integral performance of accident tolerant fuel designs under normal and transient conditions and to demonstrate improvements under severe accident conditions. For this reason, system codes like RELAP5 [212], RELAP5 -3D [221,226], and PWR severe accident analysis code MIDAC [227] are also modified. Finally, multi-scale models are expected to play important roles in ATF R&D by reducing the need for in-pile testing and accelerating the safety review process. For example, molecular dynamics and phase field methods have been used to predict irradiation degradation of U–Mo and SiC composite cladding [228,229].

3.2. Implementation of advanced modelling techniques

3.2.1. Multi-scale developments

Traditional fuel performance codes employ continuum mechanics techniques at the macroscopic scale, where both the granular and atomic nature of the materials is ignored. The microstructure of the fuel and cladding materials, including the presence of inhomogeneities (such as Pu-rich agglomerates in MOX fuel) and defects (such as grain boundaries and dislocations) is also usually treated in only a basic manner.³ Microstructural features are typically only modelled explicitly in the determination of fission gas swelling and release using classical techniques to simulate diffusion of fission gas between features, and migration and interactions of the features themselves. The SFPR code arguably represents the state of the art in this context, with intra-granular fission gas bubble nucleation, growth, migration, coalescence, interactions with dissolved gas, dislocations and vacancies, thermal

re-solution and irradiation-induced re-solution all modelled [84].

Given the deficiencies in traditional fuel performance codes described in the paragraph above, there is a drive for multi-scale modelling to be applied to fuel performance, where modelling techniques at different length scales are employed and combined to better simulate fuel behavior under irradiation [230–234]. The aim is to provide a more theoretical, and less empirical, basis for fuel performance modelling, thereby allowing extrapolation of material behavior to conditions outside the validation range, and enabling more generic application to novel fuel designs with non-standard materials. At the electronic scale, density functional theory is being used to predict basic properties of materials (for example, lattice structure) and to provide potential functions (potential energy as a function of separation of two atoms) for use in higher-scale modelling [235]. At the molecular scale, molecular dynamics is being used to predict material thermophysical properties and to simulate the effects of irradiation-induced damage on the microstructure and hence on the thermophysical properties [235]. At the mesoscale (that is, the scale of microstructural features), dislocation dynamics, cluster dynamics, kinetic Monte Carlo methods and the phase field approach are being used to simulate the evolution of the microstructure with time [235]. Finally, at the macroscopic scale, the finite element method, the finite element cohesive zone method [236], the extended finite element method (XFEM) [237], peridynamics [235,238], the discrete element method [239,240] and smooth particle applied mechanics (SPAM) [241] (also commonly referred to as smooth particle hydrodynamics, SPH) are being used to predict the solid mechanics. These are being used in particular in an attempt to more accurately simulate the behavior of cracked and fragmented materials, and to model the cracking and fragmentation processes themselves. Promising results from peridynamics and the discrete element method are illustrated in Fig. 7, Fig. 8 and Fig. 9.

Much of the multi-scale modelling performed so far has been done separately from other efforts, with no integration of modelling at different length scales attempted due to the technical and computational difficulties associated with such coupling, not to mention the validation issues. Thus, for example, thermophysical properties predictions from lower-scale modelling have in general been used to generate material property models in fuel

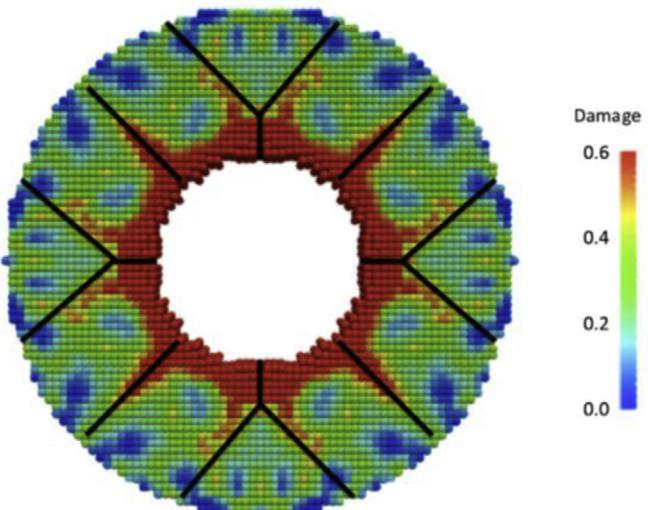


Fig. 7. Peridynamics predictions of damage fraction (fraction of bonds between particles that are broken) for a 2-D slice of an AGR fuel pellet ramped to 15 W/g (modelled using a particle-based implementation of peridynamics in the LAMMPS molecular dynamics code; black lines are overlaid to show approximate locations of cracks) [238].

³ There are some exceptions for heterogeneous materials. For example: (a) in recent CYRANO developments for MOX fuel, fission gas and helium generation and release in each of the different phases are modelled explicitly, and micro-mechanical behavior laws are being implemented to evaluate the local stresses and strains in each phase [119] R. Largentot, K. Audic, F. Douchin, C. Pétry, “CYRANO3 the EDF fuel code performance: global overview and recent developments on MOX fuel”, Proceedings of TopFuel 2016, ANS, Boise, ID, USA, 11–15 September 2016, p. 621.; and (b) in ALCYONE, the so-called FE² method has been implemented to perform thermo-mechanical analysis at both the macroscopic and microscopic (local heterogeneity) scale using consistent macroscopic and microscopic finite element meshing [121] V. Marelle, P. Goldbronn, S. Bernaud, E. Castelier, J. Julien, K. Nkonga, L. Noirot, I. Ramière, “New developments in ALCYONE 2.0 fuel performance code”, Proceedings ofibid., p. 643.

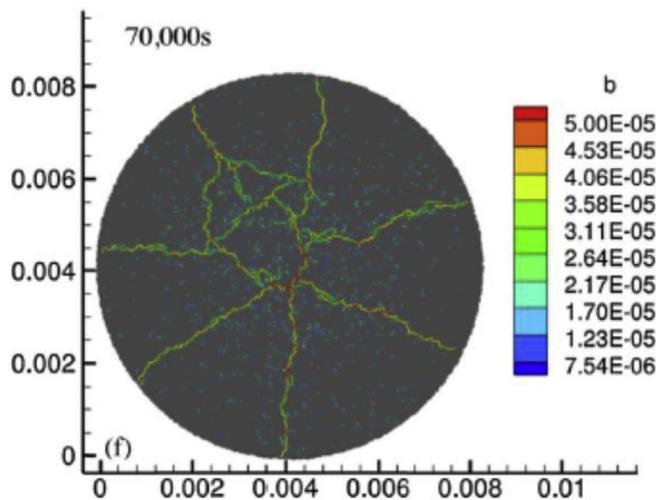


Fig. 8. Discrete element method predictions of the crack pattern and crack aperture width (colours; units are metres) for a 2-D slice of a PWR fuel pellet after two cycles from zero power to 25 kW/m and back to zero power [239]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

performance codes, rather than to generate property predictions ‘on the fly’. (A notable exception is the coupling of MARMOT – a MOOSE-based code employing the phase field approach [242] – and BISON to evaluate fuel thermal conductivity [243], although this was only a proof of concept, without accurate modelling of the underlying physics.) This is likely to change in the future given advances in computing power and experimental techniques, as well as the international momentum behind the multi-scale modelling paradigm.

3.2.2. Multidimensional developments

As described above, most LWR fuel performance codes like FRAPCON [66,161,162], ENIGMA [104,148,244,245], TRANSURANUS [109,246,247], etc. represent the cylindrical fuel rod using a 1.5D geometrical approach. Notable exceptions include FALCON [68,248] which is 2D and ALCYONE [89,249,250] and BISON [70,92,243], which can be either 2D or 3D. Validation studies [245,246,251] demonstrate that the 1.5D approximation is reasonable and efficient for simulation of smeared fuel (i.e., the pellet stack is considered a single cylindrical body) where the geometry and boundary conditions can be assumed to be axisymmetric.

Cases exist, however, where higher dimensional analysis is important. Examples include: 1) non-axisymmetric fuel geometry (e.g., defective pellets or nonconcentric pellet alignment), 2) interest in discrete pellet behavior (e.g., pellet cracking or variation in pellet dish geometry due to fuel creep), or 3) non-axisymmetric

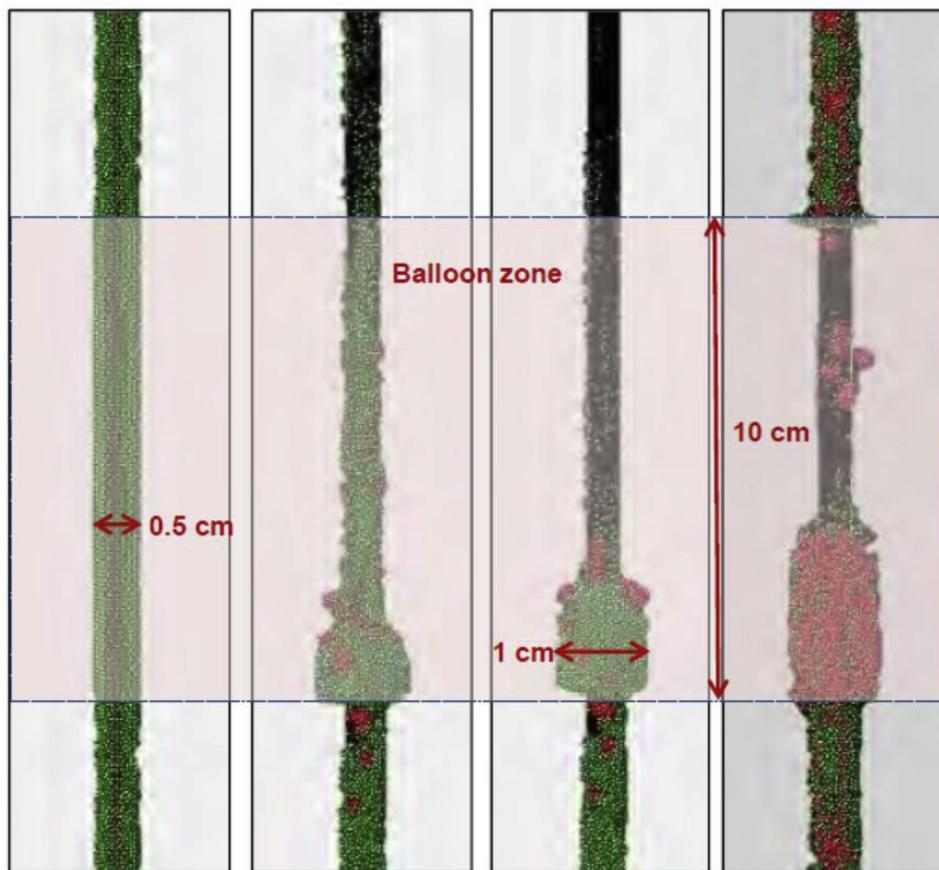


Fig. 9. Discrete element method predictions of the axial re-distribution of small and large fuel fragments (green spheres and clusters of red spheres) during a LOCA event with cladding ballooning (the cladding tube is not shown; the three leftmost images provide snapshots at the beginning, middle and end of a simulation; the rightmost image is a snapshot, close to the end of the simulation, of another simulation with a greater number of large fuel fragments) [240]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

boundary conditions (e.g., azimuthal variation in clad wall temperature). For such cases, a variety of approaches are taken, for example:

- 2D Cartesian geometries used to study the fuel rod cross section containing non-axisymmetric geometry or boundary conditions [252,253].
- Localized 2D or 3D analyses, in which only a single pellet, section of pellet, or short segment of a full rod is considered [179,243,254–257].
- Combined analyses, in which 1.5D or 2D-RZ models are used to analyze full rod behavior and provide time-dependent boundary conditions for detailed 3D submodels [258].

It is noted that 3D analysis of every fuel pellet in a full-length fuel rod requires highly parallel computing capability and substantial computing resources. Although such detailed analyses are rarely necessary, modern codes such as BISON [243] hold promise for such calculations.

3.3. Code coupling for multi-physics simulations

Current efforts to integrate or merge fuel rod behavior modeling tools dealing with different operation conditions such as FRAPCON4.0 and FRAPTRAN2.0 [259], or FEMAXI and RANNS [260] should be briefly mentioned first. They are driven by the wish to simplify the development, maintenance and use of the fuel performance code to simulate the fuel behavior under all operating conditions. This follows extensions of fuel performance codes for normal operating conditions (including anticipated transients) to include models and material properties for dealing with design basis accidents such as LOCA, or storage conditions. This was the case for the TRANSURANUS code [261] starting with the EXTRA project [262], and has recently been launched for the BISON code [263]. Likewise, codes or models that were traditionally conceived to simulate nuclear fuel behavior under accident conditions, specifically MFPR [87] and TESPA, have been extended to full rod codes, SFPR [86] and TESPA-ROD [264,265] respectively. These can also handle normal operation as well as storage conditions.

A lot of attention has also been given to coupling of codes in order to obtain a multi-scale and multi-physics simulation tool for reactor safety analysis, in which fuel performance codes play a crucial role. With the advent of advanced hardware and software over the past two decades, state-of-the-art coupled code systems have been developed. This started with greater detail in neutronics and thermal hydraulics modelling. Code coupling gradually replaces a sequence of separate but conservative analyses by means of individual code calculations for different domains, such as sub-channel thermal hydraulics (including CFD), reactor dynamics and thermal hydraulics system codes. These typically contain either a simplified fuel behavior model or a set of fuel rod parameters provided as input tables by a fuel rod performance code (e.g., gap heat transfer coefficient). However, current fuel performance codes have made great progress in describing the fuel behavior at high burnup during normal operation as well as under design basis accident conditions (DBA) over the last two decades. This constitutes the driving force for evaluating the potential benefit resulting from replacing simplified fuel behavior models in the above mentioned system codes by means of a two-directional coupling with a fuel performance code.

In the past few years, a one-way coupling approach has been developed for a whole core analysis. SIMULATE-5 from Studsvik provided input to the ENIGMA fuel performance code [266]. A two-way coupling approach was also developed by JNES for the FEMAXI code and the thermal hydraulics system code TRACE in the frame of

the benchmark of the OECD-NEA [265] for RIA. Similarly, the transient fuel performance code FRAPTRAN was coupled in two directions with the thermal hydraulics model GENFLO from VTT [267]. For example, GENFLO provided the axial power profile and thermal hydraulics conditions to FRAPTRAN on one hand, while the fuel performance code returned the gap conductance and the flow area reduction due to ballooning on the other hand. More recently, KAERI launched the development of the coupled FRAPTRAN code (using burnup-dependent variables from FRAPCON) with the MARS system code that provides the thermal hydraulic boundary conditions for a LOCA analysis in the frame of the FUMAC CRP of the IAEA [268].

In parallel to this, different coupling efforts have been made involving the TRANSURANUS code with various other simulation tools. For that purpose, a more general interface for direct coupling of the fuel performance code with other codes (including thermal-hydraulic system codes such as ATHLET, sub-channel codes such as SubChanFlow or the reactor dynamics code DYN3D) was developed first but was not distributed [269]. Therefore, KIT developed its own direct coupling scheme of TRANSURANUS with the PARCS and SubChanFlow codes [270], whereas Lappeenranta University developed a coupling of the TRANSURANUS code with the SERPENT code of VTT as part of Euratom's ESSANUF project [271]. The coupling with this Monte Carlo code is somewhat particular and aims to more accurately simulate fuels doped with absorbing materials, since fuel performance codes usually adopt a diffusion based solution, which is not accurate in the presence of strong absorbing isotopes (see "Neutronics modelling"). Finally, the coupling of the MFPR code with TRANSURANUS has also been launched recently in collaboration with IRSN [181]. The detailed mechanistic models of MFPR should provide an improved tool for the prediction of fuel rod and fission product behavior under normal, off-normal or accident reactor conditions (up to the temperature for which cylindrical fuel geometry will be kept) as well as for fuel storage and reprocessing facilities. Being physically informed and more predictive, this code should also be able to act as a reference fuel performance or safety and source term tool in various conditions.

In addition to the coupling of individual tools directly, platforms have also been developed for code coupling over the last decade. For instance the European NURESIM platform [272], based on SALOME, has been developed in the frame of three successive Euratom projects with more than 22 organizations. It is a generic open source platform that includes pre and post-processing for numerical simulation mainly developed by CEA, EdF and OPEN-CASCADE [273]. In a first step, the SCANAIR code of IRSN for RIA simulations has been integrated. As part of the current McSAFE project coordinated by KIT, both the TRANSURANUS and the new FINIX tool [274] (under development by VTT) are being integrated. This will not only enable a more general coupling in an open-source platform, it will also ensure legacy codes originally developed in Fortran such as TRANSURANUS, can run in a modern environment by means of the specific interface for code coupling. One can thus integrate its own numerical solver for fuel performance as a component (C++ or Python) and be coupled with other codes developed in C++, for example.

Similarly, in the USA, MOOSE (Multiphysics Object Oriented Simulation Environment) has been developed and distributed by INL as an object-oriented C++ finite element framework for the development of tightly coupled multiphysics solvers [275]. It currently contains more than 20 applications such as the BISON fuel performance code [44] and the MARMOT finite-element-based phase field code [242] for modelling irradiation-induced microstructure evolution. It is also being used by industry, research centers and universities - for example as part of the CASL and NEAMS projects.

3.4. Uncertainty analysis and sensitivity analysis

3.4.1. Which UA/SA

Uncertainty and sensitivity analyses complement the outcome of the simulation tools applied for safety analysis or the design of nuclear fuels in view of our lack of knowledge about physical phenomena as well as imperfect experimental data. In order to assess the technological impact or the propagation of all sources of uncertainties in fuel performance modelling (e.g. centerline temperature, internal gas pressure, cladding strain), different techniques can be considered.

So-called sensitivity methodologies may involve straightforward multiple runs with varying input data and/or model parameters, or could rely on a more rigorous treatment such as perturbation theory, although this is usually not applied to fuel rod modelling because of the challenges to formulate all differential equations corresponding to non-linear phenomena. One example is the numerical noise technique that was included in the TRANSURANUS code in 1980 [276], allowing the evaluation of the standard deviation of the center temperature for example in one single run. To this end, it is sufficient to apply random deviations in a small interval (numerical noise) to the most important fuel rod parameters such as the linear heat rate. By analyzing the resulting changes in the relevant output (e.g. center temperature) one can infer the corresponding sensitivity of the code to input parameters of interest. However, while the computational effort is equivalent to one single deterministic run it is impossible to extract directly information about the influence between different uncertain parameters.

Another class of probabilistic methods, used in experimental design for example, is the response surface technique. Concrete examples include the Latin hypercube sampling or the Taguchi experimental design, whereby a combination of varying input parameters is carefully selected, and this has been tested with the FRAP code by Peck [277]. The main disadvantage of such an approach is that one has to determine in advance which parameters should be varied and by how much. Furthermore, the interactions between the modified parameters must be also defined, although this may not be straightforward.

The Monte Carlo method is also applied relatively often in the nuclear field. Its application to nuclear fuel rod calculations relies on random sampling of all variables considered and is straightforward, hence attractive. Nevertheless, the large number of cases involved implies a high computational cost and it also implicitly requires the knowledge about the variable distributions that may not be well characterized. Furthermore, the outcome usually does not allow disentangling the individual contribution of each uncertain input parameter. In order to reduce the computational burden, quasi-Monte Carlo methods have been considered for the STAV6 code for example [278]. They combine the variations of parameters in response surface techniques with the standard Monte Carlo method. As a result, the quasi-random sampling sequences fill the variable space more uniformly compared to random numbers. Despite the restrictions and lack of consensus, applying a limited variation of some fabrication parameters in fuel rod calculations is being considered in Germany [279–281] and the USA [282] for two reasons. The first driving force stems from the hope to better quantify (and reduce) the degree of conservatism. For this purpose, some advocate [281] the replacement of a deterministic calculation with the worst case dataset, i.e. with a superimposed unfavorable tolerance limit on some fabrication parameters, by means of probabilistic calculations. The second argument relies on the observation that some probabilistic simulations sometimes provided worse performance predictions compared to the deterministic, so-called worst-case simulations. Of course, this will be

determined by the proper definition of the worst case and will depend on the limits of variation applied in the probabilistic method.

A semi-statistical design approach has therefore been suggested in Germany [279,280]. It is based on Spearman's rank coefficients that can be inferred from a limited number of Monte Carlo simulations.

In order to obtain a set of parameter combinations that provides a fuel response (e.g. fuel center temperature) covering with a given probability the total output range when applying all possible parameter combinations, the rank coefficients are converted into quantiles of the statistical distributions. In a similar manner, a non-parametric order statistics method based on Wilks' formula derived from the tolerance interval method is being applied in the USA [282], and more recently also in Finland with the FRAPTRAN-GENFLO code [283]. The methods provide a more realistic evaluation of the operational margin. This is accomplished through the statistical evaluation of numbers of fuel rods coming close to the design limit by assessing the statistical certainty for the actual occurrence of extreme cases.

3.4.2. How to implement the UA/SA

The application of uncertainty and/or sensitivity analysis to fuel rod performance codes can be considered and is developed in three different ways. The first, most straightforward manner is to couple the fuel rod performance code with a statistical package such as DAKOTA or URANIE. This has been tested for the FRAPCON [284], PAD5 [285] and BISON [286] codes with DAKOTA, for METEOR with URANIE [287]. Such an approach demands development of an interface between the fuel simulation tool and the statistical package. It also requires considerable computational power as well as storage capacity, not to mention the processing time of all output files by the statistical package afterwards. A second approach consists of writing a statistical wrapper around a fuel performance code with a graphical user interface, as was applied for TRANSURANUS by NINE [195] and by VTT for the ENIGMA code [215]. This is usually more tailored to the specific needs or scope of the user. In a similar way, the third approach consists of implementing statistical abilities in the fuel performance package, which requires much development but enables much faster analysis in comparison with the first approach where many file access operations are required. Such an approach was adopted in 1980 in the TRANSURANUS code [276], and gradually extended over time [288,289]. A new graphical user interface has recently been developed for this [196]. Future developments are intended to extend the number of possible uncertain input parameters and to apply other sensitivity analysis methods, as well as to use statistical software for parameter optimization and calibration (e.g. with DAKOTA [285]). However, the biggest challenge at the moment is to reach consensus about how UA/SA should be applied for each case, in each country. A first attempt to reach such consensus was made during the second phase of the RIA benchmark organized by the OECD-NEA, wherein all participating codes and corresponding approaches are summarized [290].

4. Code verification and validation

Beginning at inception, the development, verification, and validation of a code must be carried out following rigorous quality procedures [291]. The verification and validation of fuel performance codes is usually organized in three main steps [44,246,250]. The first step consists of verifying the correctness of the mechanical–mathematical framework. Sometimes it is referred to as code verification, while solution verification includes a quantitative assessment of the numerical accuracy of a given solution for a

problem. For this purpose, when exact (analytical) solutions are available they are compared with individual models from the code. The numerical analysis of the individual model can also be optimized by testing various solution techniques (e.g. for intergranular diffusion in a sphere). The second step consists of an extensive validation of individual models from the fuel performance code by means of comparison to separate-effect data. The last step in the validation process relies on a comparison with integral experimental data, and is sometimes complemented by a code-to-code evaluation (e.g. in the frame of international benchmarks as mentioned below). The different sources of experimental data are outlined in the next section.

In the present paper, which is limited to LWR fuel, we will adhere to those steps rather than giving a separate overview for each type of fuel (UO_2 , Gd -doped UO_2 and MOX). Moreover, it is beyond the scope of this paper to provide details about the validation of each code in the open literature. As will be clarified in the next section summarizing the experimental data used for validation, this is mainly because of the variable amount of experimental data available for each type of fuel, but also because of the varying scope of each fuel performance code. Furthermore, we limit ourselves to the two steps of validation. Readers interested in the first step are referred to Refs. [54,72,292–295] as examples mainly dealing with the validation of the numerical temperature, fission gas release calculation or mechanical analysis. A following section outlines and analyses the validation of the sub-modules or models in the codes. Then, a summary is provided of the integral verification process of the fuel performance codes under both normal operating conditions and design basis accidents such as the loss of coolant accident (LOCA). The final section outlines the main challenges.

4.1. Data used for validation

Experimental information for integral validation of fuel performance codes can be globally categorized as public or proprietary data. Obviously, the second category cannot be considered here, even though it represents the major part for fuel rod codes developed by industry (e.g. Refs. [117,175]) and comes from their surveillance programs. In view of the required time and resources for establishing such a database, many (research) organizations often take part in international projects making use of experimental reactors. Such tests usually involve several steps: base irradiation in either a test reactor or a power reactor, followed by the experiment itself in the test reactor, sometimes interrupted by intermediate non-destructive analysis, and finally both non-destructive and destructive post-irradiation examinations in hot cells. An overview of the main international programs conducted on LWR fuel from 1970 to today is included in Table 2.

Fuel testing started in the early 1960s. The world's first LWR MOX fuel irradiation campaign for example, started in 1963 in the BR3 PWR reactor of SCK-CEN with fuel manufactured from Belgo-nucleaire. For more than 18 years, these two organizations jointly managed international programs supporting MOX utilization in LWRs [296]. Other European national experience with MOX fuel in commercial LWRs started in the same period (e.g. in Germany in 1966 and Italy in 1968) and was reviewed by Brown et al. [182] in 1999.

As summarized by Grounes et al. [297,298], Studsvik Nuclear also managed a long series of both bilateral and international fuel R&D projects primarily addressing the PCI/SCC failure phenomenon in conventional fuel rods since the early 1970s. In these tests, fuel rods and rodlets were irradiated in a variety of reactors under prototypic conditions before being shipped to Studsvik and testing in the R2 reactor. These tests provide a comprehensive data set on

PCI failure propensity in BWR and PWR fuel under a variety of ramp conditions. Data are also available about fission gas release for rods that sustained ramping without failure. More recently SCIP projects were organized by Studsvik, with a stronger focus on the high burnup phenomena such as the hydrogen assisted cladding failure modes during PCI/PCMI [299].

In parallel to the above mentioned activities, Risoe national laboratory in Denmark carried out three main irradiation programs aiming at studying fission gas release and microstructural changes during slow ramp tests with holding time, referred to as bump tests [300,301].

In the USA, the series of EPRI-led Nuclear Fuel Industry Research (NFIR) Programs started in the 1980s. These aimed to generally improve fuel reliability and performance by acquiring basic knowledge of the in-reactor behavior of fuel, cladding, control materials, and other core components.

In Japan, research for the analysis of the underlying mechanisms involved in the HBS was carried out in the 1990s as part of the HBRP [46–49], HRBP_NT [35] and NXO projects [302,303]. More specific research for fuel safety under design basis accidents has been carried out in the NSSR under the ALPS projects [304].

In the above mentioned projects, initial tests were carried out with fresh fuel in dedicated research reactors. With the strong development of in pile instrumentation and fuel rod re-fabrication, thanks in particular to Studsvik, Risoe and the OECD Halden Reactor Project [310], the access to integral experimental data has made a great leap forward and cumulated in the Halden database. A great deal of useful data have been generated and were used for code development, validation and benchmarking by most fuel performance code developers. An excellent review of nuclear fuel experimental data from the IFE-OECD-Halden Project was published in 1995 by Turnbull et al. [311].

In view of the non-negligible costs for participation in such projects, and also because of concerns about knowledge management, the idea of generating the International Fuel Performance Experiments database [312] was raised in 1995 [313] and it was established in 1998 [314], thanks to collaboration among main international organizations (IAEA, OECD-NEA and the OECD Halden Reactor Project). This database has continuously been expanded and improved, and has played a key role in the recent international fuel performance code benchmarks. From the start, the objective has been to cover data from as many reactor systems as possible. Currently, information from PWR, BWR, VVER and CANDU fuel is included. Discussions are ongoing to extend the database with fast reactor fuel experiments (see Integral code validation and benchmarking below).

4.2. Validation of submodels

Any fuel performance code combines many material properties for the fuel, cladding, fill gas and coolant, as well as individual models for other considerations such as isotope evolution or fission gas behavior. In the following, we will refer to these as submodels and limit ourselves to discussing the use of experimental data for their validation as the first step of the code validation process. It should be noted, however, that not necessarily all submodels can be validated separately; hence, we restrict ourselves to those for which information is available in the open literature.

4.2.1. Radial power

As addressed in the section entitled "Neutronics modelling", the radial power distribution is of primary importance for fuel performance simulations, since it provides the source term for both the calculation of the temperature distribution and the (radioactive) fission product distribution in the fuel.

Table 2List of the main international programs conducted on LWR fuel (UO_2 and MOX) since 1970.

Project	Period	Subject	References
INTER-RAMP	1975–1979	BWR (10–20 MWd/kg) Failure threshold and mechanism	[297,298]
OVER-RAMP	1977–1980	Failure threshold, design parameters	[297,298]
DEMO-RAMP I	1979–1982	PCI remedies with annular, niobia-doped pellets	[297,298]
TRIBULATION	1984–1987	Fuel rod behavior after an accidental transient	[305]
HBEP	1979–1988	Fission gas release at high burnup and high burnup fuel transformation (HBS)	[306]
DEMO-RAMP II	1980–1982	Failure threshold for PCI during short time power transients with eight pre-irradiated BWR rods	[297,298]
SUPER-RAMP	1980–1983	16 BWR and 28 PWR rods, failure threshold, high-burnup effects, PCI remedies, safe ramp rate and Cd-doped fuel	[297,298]
SUPER-RAMP EXTENSION	1984–1986	Safe ramp rate with nine BWR rods, and resolve unexplained failure resistance with four PWR rods	[297,298]
TRANS-RAMP I	1982–1984	Failure boundary, crack initiation and propagation, structural changes, fission gas release in BWR fuel	[297,298]
TRANS-RAMP II	1982–1986	Failure boundary, crack initiation and propagation, structural changes, fission gas release in PWR fuel	[297,298]
SUPER RAMP II 9 × 9	1987–1990	PCI performance in four BWR rods	[297,298]
NFIR I	1982–1988	Global fuel behavior at high burnup	[35]
DOMO	1985–1996	Fission gas release and microstructural changes in 10 MOX and five UO_2 BWR fuel rods	[307]
ROPE I	1986–1993	Clad creep-out as function of rod overpressure in 4 BWR rods	[297,298]
HBC	1987–1994	High burnup fuel chemistry	[35]
PRIMO	1987–1994	Fission gas release and microstructural changes in 15 MOX PWR fuel rods	[182,307]
NFIR II	1988–1994	Fuel rod behavior under irradiation, fuel and cladding properties	[35]
TRANS-RAMP IV	1989–1994	Influence of non-penetrating cracks on PCI failure in seven PWR rods	[297,298]
ROPE II	1990–1994	Clad creep-out as a function of rod over-pressure in six PWR rods	[297,298]
NFIR III	1992–1999	Fuel rod behavior under irradiation, fuel and cladding properties	[35]
DEFEX	1993–1995	Secondary damage formation in fuel rods with simulated fretting defects in six fresh BWR rods	[297,298]
FIGARO	1994–2000	Fission gas behavior and thermal behavior of two re-instrumented MOX PWR fuel rods	[182,307]
HBRP	1994–2002	HBS study	[46–49]
DEFEX II	1995–1997	Same as DEFEX II with six irradiated BWR and PWR fuel rods	[297,298]
NFIR IV	1998–2004	Fuel rod behavior under irradiation – fuel and cladding properties	[35]
ALPS	2002–2010	Behavior of high burnup fuels under accidental conditions (RIA and LOCA)	
HBRP_NT	2002–2007	HBS study	[35]
NFIR V	2004–2010	Fuel rod behavior under irradiation, fuel and cladding properties, fuel dispersion	[35]
NXO	2006–2010	Multiscale approach of HBS	[302,303]
SCIP	2004–2009	PCI/PCMI and hydrogen-assisted cladding failure modes	[299,308]
F-BRIDGE	2008–2012	Acquisition of basic data for modelling and multiscale approach	[232]
SCIP-2	2009–2014	Continuation of SCIP, stress corrosion and hydrogen-assisted fracture mechanisms, and propagation of cladding cracks	[309]
SCIP-3	2014–2019	LOCA and off-normal temperature transients	[309]
ALPS II	2014–2019	Behavior of fuels with advanced materials under design basis accident conditions	[304]

The direct assessment of the radial power distribution relies on the radial profiles of fission products and fissile atoms obtained from post irradiation examination by means of either EPMA or SIMS (e.g. Ref. [315]). More precisely, the radial distribution (or even better the two-dimensional mapping) of Pu, Nd, Gd, etc. can be directly compared with the values provided by a submodel for nuclide evolution. Since in thermo-mechanical fuel performance calculations the absolute value of the generated power is input data, only the relative radial power profiles need to be calculated and the models can be validated on normalized radial distributions of actinide concentrations obtained by means of EPMA, SIMS, or by means of Monte-Carlo burn-up code computations such as ALEPH or VESTA [316]. In Fig. 10, the normalized burn-up and plutonium

profiles predicted by TUBRNP for UO_2 fuel with a burn-up of 102 MWd/kgHM are in excellent agreement with the EPMA-measured values of Walker et al. [96]. Likewise, for VVER fuel the TUBRNP predictions match well with the EPMA results at a burn-up of around 60 MWd/kgHM [125]. The shape of these radial profiles is rather independent of the power history, i.e., on the path to accumulate a given burn-up level.

The radiochemical analysis of samples taken at various radial positions in a fuel pellet, or their analysis by means of evaporation in a Knudsen Cell that is coupled with a mass spectrometer (KC-MS), can also be considered for the validation of a sub-model such as RADAR or TUBRNP (e.g. Ref. [123]). Indeed, the analysis provides an accurate determination of element concentrations that cannot

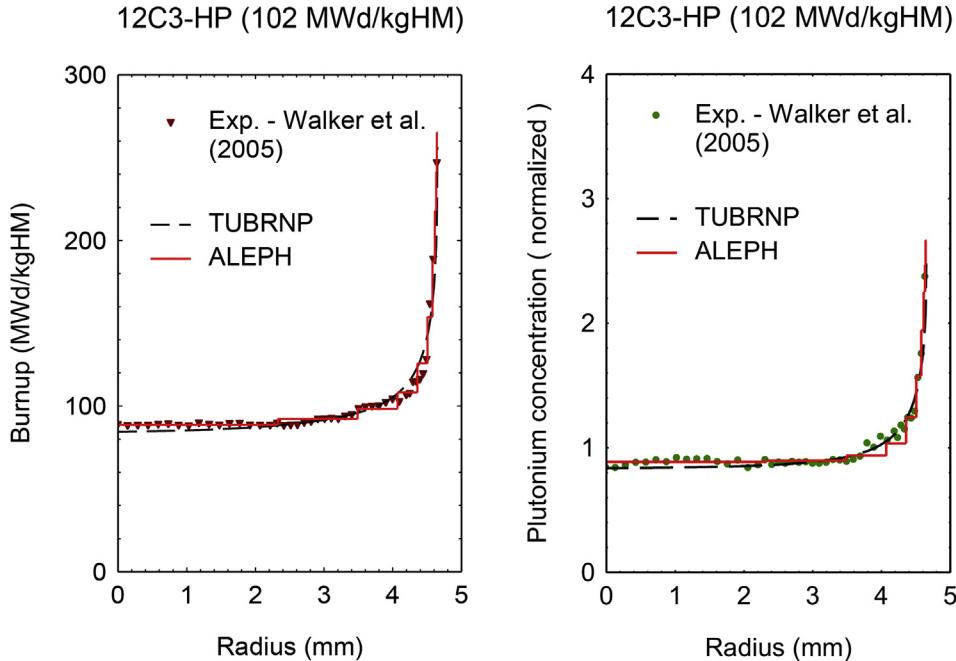


Fig. 10. Radial distribution of the local burnup (left) and the normalized Pu content (right) calculated by TUBRNP and ALEPH and compared with EPMA results at very high burnup [123,316].

be measured by means of EPMA or SIMS, albeit with a much lower radial resolution (especially for samples close to the pellet outer radius in high burnup samples). In the case of the KC-MS there can be an additional uncertainty about the stoichiometry evolution during the (non-congruent) evaporation phase.

Further needs for PIE data in the open literature for the validation of radial power profiles are related to absorbing doped fuels such as Gd-doped oxides or innovative fuels such as thorium based oxides or inert matrix fuels for LWRs [194], for which data are scarce, and therefore sometimes complemented with more detailed Monte-Carlo burn-up code computations as mentioned above. Additionally, there is a need to obtain experimental data up to higher discharge burn-up values for MOX fuel, for both MIMAS and SBR types in order to account for the difference in the micro-structure brought about by the various industrial fabrication processes.

4.2.2. Gap conductance

The heat transfer in the fuel to cladding gap corresponds to a combination of three different heat transfer mechanisms: transfer via convection and conduction in the gas-filled gap, via direct contact points when the gap closes, or via radiation when the temperatures are high enough. Such an evaluation cannot be derived from PIE as it would obviously require an accurate and simultaneous measurement of the heat flux, the temperature difference across the gap and the (azimuthal) average gap distance. Moreover, the gap size is affected by most phenomena occurring in the fuel (thermal expansion, swelling, densification, creep, cracking and relocation, etc.) and cladding (thermal expansion, creep down, etc.) and cannot be measured accurately online. Finally, conventional fuel performance codes consider azimuthal symmetry, hence an average gap size, although it is obvious that pellets undergoing cracking at the first rise to power will not necessarily perfectly align in the center of the rod. The average gap size and the gap heat transfer coefficient assessment are therefore subject to large uncertainties.

Nevertheless, a specific technique has been developed at the OECD Halden Reactor Project that allows axial and azimuthal assessment of the averaged gap size during irradiation. To this end, gas lines have been connected to instrumented fuel rods, which enable the gap size assessment thanks to so-called hydraulic resistance measurements when flushing a known quantity of gas through the rodlet in a specific time interval. Furthermore, center temperature measurements obtained by means of thermocouples or expansometers at beginning of life are used to verify the gap conductance and/or models for fuel cracking and relocation. The gap conductance models should thus be able to reproduce the effect of gap size and gas composition and pressure as faithfully as possible, provided that the effect of densification can either be minimized (e.g., by using very dense material to start with) or measured via stack elongation measurements during standby. Turnbull reviewed the data from the Halden reactor in 1995 [311]. The validation of the URGAP model for the gap conductance of the TRANSURANUS code is one example for using such data [43]. This is done either as direct comparison of central temperatures as a function of the variation of gas composition for instance, or as the indirect estimation of the gap conductance derived from the temperature measurements. Similar measurements and validation work were carried out in France [39,317].

4.2.3. Thermal conductivity

As explained in section Thermal performance, the heat transfer in the fuel mainly occurs by means of conduction, although there are exceptions such as thorium dioxide that are semi-transparent for heat transfer by radiation. It is thus necessary to verify the model for the thermal properties, in particular the thermal conductivity. This is typically based on experimental data from out-of-pile tests [7,318,319], as illustrated in Fig. 11.

To summarise the figure, the predictions of the thermal conductivity match fairly well with the experimental values obtained by Ronchi and co-workers [7] by means of laser flash measurements on fresh and irradiated fuel. Nevertheless, there are

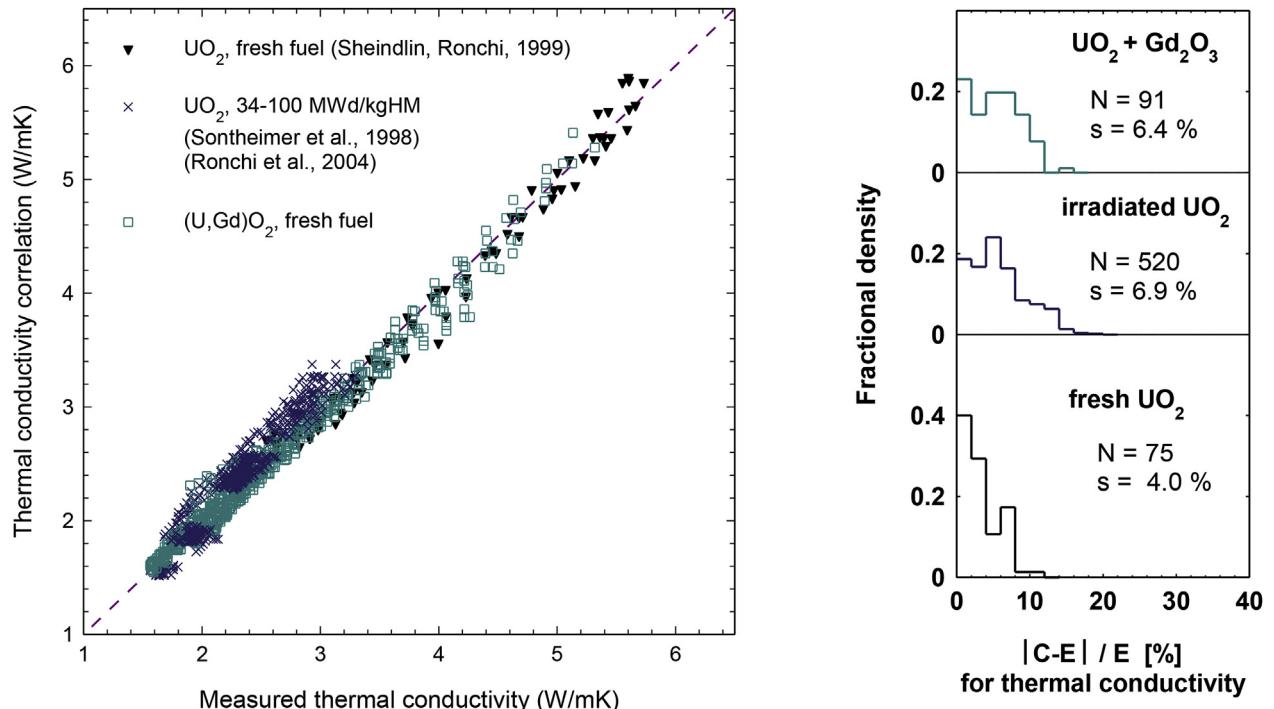


Fig. 11. Comparison of experimental thermal conductivity values with predicted values obtained by means of the model in TRANSURANUS for UO_2 and $(\text{U},\text{Gd})\text{O}_2$ fuel.

remaining open questions and therefore, a need for experimental data to disentangle the separate effects of plutonium concentration, (local) stoichiometry deviations, minor actinide additions and burnup effects in mixed oxide fuels. This can be complemented with more detailed simulation tools, such as in the recent molecular-based analysis of UO_2 [320] and MOX [321].

4.2.4. Elastic and plastic properties

Experimental data relating the mechanical properties of (irradiated) UO_2 to its local microstructure are of practical importance to ameliorate the understanding of how (high burnup) fuel properties can affect the pellet-cladding interaction. Among several structural factors that affect the fuel mechanical properties (e.g., accumulation of radiation damage, porosity, grain size, and local deviations from stoichiometry) apart from the temperature, the porosity is thought to play a major role while reducing the load-bearing area, especially in the HBS. The highly heterogeneous character of the irradiated fuel microstructure along the pellet radius makes the experimental investigations difficult. The traditional mechanical testing methods for nuclear fuel rely therefore on micro-indentation (e.g. Refs. [76,77]) or more recently on high-frequency acoustic microscopy [79,81,322]. They enable a satisfactory analysis of Young's modulus as a function of the burnup [77], as used in fuel performance codes today. More recently, Terrani et al. [78] have expanded this work by means of nano-indentation, which does not need an assumption about the relationship between elastic modulus and hardness or density.

4.2.5. Cladding oxidation

The thickness of the oxide scale that develops on the coolant side of the cladding is another important limit for fuel performance. It impairs the thermal heat transfer across the cladding, reduces the thickness of the metal that can sustain stresses, and deteriorates the mechanical properties of the remaining metallic part via the amount of hydrogen absorption that accompanies oxidation. This is because it can reduce ductility by hydride precipitation, especially

when this occurs along the radial direction. Finally, clad oxidation at high temperatures is exothermic and can contribute substantially to the local heating of the cladding in the event of a LOCA.

In general, empirical correlations for the oxide thickness or mass gain are applied for each type of cladding in the specific coolant conditions (temperature, pH, Li concentration etc.) and local heat flux [323]. Out of pile measurements of oxide thickness can be obtained by means of eddy current measurements. Nevertheless, they are rarely provided in the open literature. Even if they are, they are subject to large uncertainties due to the lack of knowledge about the coolant chemistry, irradiation history, and other considerations. It is, therefore, not very meaningful to compare the predicted oxide layer thickness of a fuel performance code with a measured axial profile in the absence of the relevant water chemistry, clad composition and microstructure (which is fabrication route dependent). Nevertheless, a number of specific rigs have been commissioned in the Halden reactor for subjecting fresh and pre-irradiated fuel rods to PWR or BWR conditions with well-controlled conditions; these experiments were reviewed by Turnbull [311]. The oxide thickness measurements rely on high-frequency eddy current probing in the reactor hall at regular intervals.

For cladding oxidation under accidental conditions, much more data have been generated in the public domain. In the 1950s, numerous experiments were carried out to assess the reaction of zircaloy with steam. Baker and Just at ANL published in 1962 [324] their conservative correlation for the total oxygen uptake, which is still used in licensing calculations today in Western countries that rely on the 1973 Emergency Core Cooling System (ECCS) Rule-Making Hearing [325]. Starting in 1974, detailed studies were also launched in Canada, Germany, Japan and the United Kingdom. This resulted in a best-estimate correlation by Cathcart-Pawel [326,327] that is still used in many codes today (e.g., FRAPTRAN and TRANSURANUS). These studies found that the weight gain, oxide layer growth and (oxide plus alpha layer) layer growth all exhibited parabolic kinetics between 900 and 1500 °C. In parallel, for the E110

alloy employed in the Russian designed VVERs, similar studies were carried out in the Russian Federation by Solyany et al. [328] and reviewed in 1995 by Bibilashvili et al. [329]. Separate effect tests on these materials were also carried out more recently in Germany [330,331] and Hungary [332,333]. More recently, in France, the zircaloy containing 1%Nb known as M5 was submitted to separate effect high-temperature oxidation tests [334,335], and the newly developed sponge-based E110 cladding tubes were also tested in the Czech Republic [336]. Summaries of all high-temperature zircaloy cladding oxidation studies up to 2009 can be found in Ref. [192] or in the state-of-the-art document of the NEA [337], which is currently under review.

Fuel performance codes have been extended to enable the simulation of design-basis accidents by implementation of specific models (e.g. clad ballooning) and material properties (e.g., high-temperature oxidation by steam). For simulating LOCA conditions in particular, specific models for the cladding-steam reaction have been derived on the basis of separate effect tests on both irradiated and fresh cladding samples. Very often, the model is based on parabolic kinetic correlations for both the oxygen mass gain and ZrO₂ layer thickness growth [338]. For example, in TRANSURANUS, the actual reaction rate constant is defined as a function of the temperature through an Arrhenius relation:

$$K_m = Ae^{-\frac{B}{T}}$$

where K_m is the oxygen mass gain rate and T is the cladding temperature [261]. A comparison with experimental data from independent experiments is illustrated in Fig. 12. Other codes are also being extended to simulate fuel rods under LOCA conditions on a similar basis, such as the BISON code [263].

The parameters in the above equation are typically obtained by least-square fitting to experimental data for the oxygen mass gain rate of different cladding materials; this should include the effect of hydrogen content [192]. Such data have been obtained in different laboratories worldwide, some of which have been included recently in the IFPE database as well [332].

4.2.6. Cladding deformation

One of the primary objectives of fuel performance assessments is to ensure that the cladding remains mechanically intact in order to prevent release of radioactive fission products to the primary circuit of the reactor. This requires reliable predictions of clad

stresses and strains. Validation of stresses is difficult as they cannot be measured online in the cladding. Therefore, the validation of mechanical models for anisotropic clad material behavior relies on the on-line monitoring or PIE of the dimensional changes in either the axial and/or radial direction, i.e. it relies on integral measurements (see “Integral code validation and benchmarking”).

Nonetheless, cladding creep tests have been carried out for the separate validation of the clad deformation model either in pile or out of pile. In-pile tests rely on the measurement of radial deformations as a function of the inner pressure. Stress is applied by internal gas pressurization of the fuel rods and diameter changes are measured online using diameter gauges. Both internal and external rod pressure are monitored online and the data are used to calculate the applied circumferential or hoop stress in the clad segments. Diameter traces are obtained by moving the gauges axially along the rods, including the end plugs. A wide range of compressive and tensile stresses should be applied to the specimens in order to infer clad creep rates corresponding to all representative conditions expected in a reactor.

As an example, Fig. 13 illustrates the comparison of the cladding creep model predictions in the TRANSURANUS code for a dedicated cladding creep experiment in a pressurized LWR loop of the Halden boiling water reactor [339].

Out of pile tests rely on the same principle, i.e. to submit cladding segments to a pressure difference under well-defined conditions (temperature, pressure, flux, etc.). The advantages of out of pile experiments (e.g. Ref. [335]) are that apart from the much smaller costs, the deformation can be monitored in greater detail. For instance, this can be done with a laser by measuring the radial deformation along the axial axis with micrometer precision, at much shorter time intervals and with better control of temperature, pressure, and oxygen and hydrogen concentrations. It is, therefore, particularly well-suited for separate-effect tests and can provide information about creep rates under most relevant conditions (including the temperature range where the alpha-beta phase transformation occurs). The main disadvantage is the absence of irradiation, which means it can only complement, not replace, in-pile experiments. The creep rate of cladding under fast neutron radiation is several times faster than that of out-of-pile tests at identical stress and temperature, and the dependency of in pile creep rate on stress and temperature is different from that of out-of-pile conditions. However, for the testing of cladding under LOCA conditions (i.e., after the reactor scram and at high

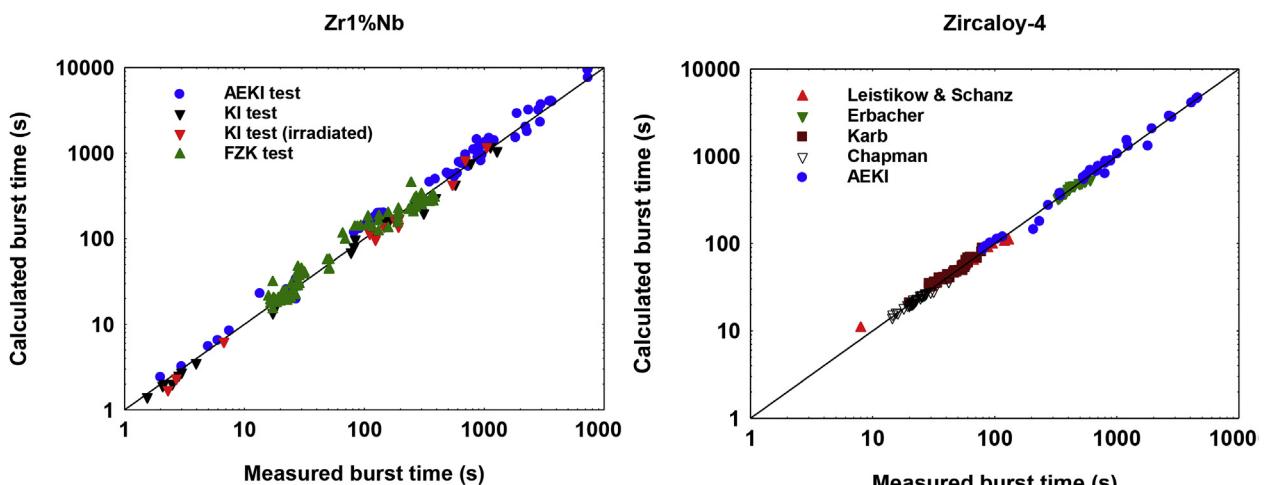


Fig. 12. Calculated versus measured time to cladding burst for Zr1%Nb (left) and zircaloy (right). Comparison of TRANSURANUS predictions and burst tests carried out with cladding tubes at the KFKI Atomic Energy Research Institute (AEKI), the Kurchatov Institute (KI) and the Forschungszentrum Karlsruhe (FZK) [262].

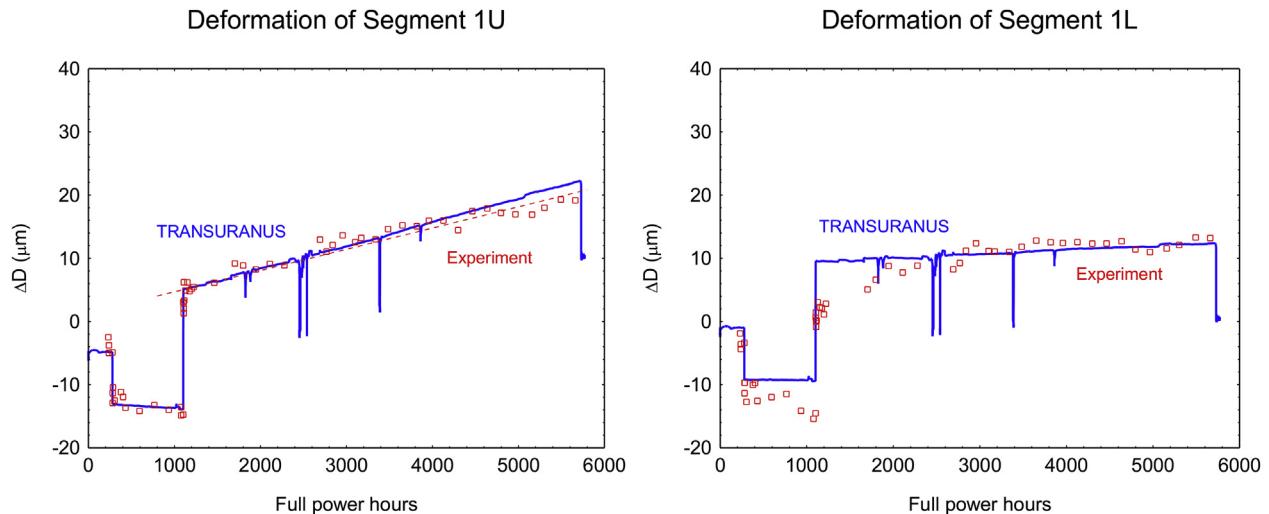


Fig. 13. Cladding diameter change of the upper (left) and lower (right) zircaloy-2 segment of Rod-1 as a function of the full power hours in IFA-663 [339]. Comparison of measured (points) and calculated data by means of TRANSURANUS (line).

temperatures such that irradiation defects can be rapidly annealed), the out of pile tests provide excellent data. Recent excellent experiments were conducted at the QUENCH LOCA facility of KIT [331], some of which have been applied in the FUMAC benchmark [340]. A complete overview of such experiments and the corresponding methodology was provided in 2009 by the NEA [337] and is under review.

Another important aspect of cladding deformation is the axial irradiation growth [341], which is a function of the fast neutron fluence and cladding type (microstructure and texture), whereas the temperature is not considered to play a major role over the typical cladding temperature ranges. A few specific tests with cladding material only have been carried out in the Halden reactor (e.g. Refs. [342,343]), but the focus is more on cladding creep. The bulk of data for irradiation growth are obtained from surveillance data in commercial plants and is therefore scarce in the open literature (e.g. Refs. [344–346] for VVER fuel rods).

4.2.7. Grain growth

Normal grain growth is only important in LWR fuel during accident conditions. The average size of the grains determines the distance that fission products and in particular gas atoms must migrate before they can be released via the tunnel network of interconnected bubbles along the grain boundaries. In addition, grain boundaries will collect insoluble fission products while they move across the fuel.

Experimental data derived from Halden experiments for equiaxed grain growth have been assessed by Palmer et al. [347] in 1986. Because of the numerous parameters that affect grain growth (temperature, porosity, stoichiometry, etc.), measurements are subject to large uncertainties. It is therefore recommended to extend and refine the available data by means of separate-effect studies. For example, a study on the basis of discs that can be submitted to irradiation or out of pile heating (by thermal resistance or laser heating) would be valuable. Out of pile heating is much less expensive and easier to combine with microscopic analysis that is needed at regular time intervals.

Making use of out of pile heating, progress in validating for example the TRANSURANUS grain growth model for UO_2 and MOX fuels was reported in Ref. [131]. The kinetics of grain growth was described by means of an expression that follows the average grain

growth in the presence of a mobile second phase (e.g. pores of an oxide), applying a kinetic coefficient K (see Microstructural changes). The 3-dimensional diameter is usually derived from the measured mean linear intercept by multiplication with an approximate factor of around 1.5 [131]. In Fig. 14 the kinetic coefficients evaluated from the present series of experiments are compared with the available data for UO_2 , revealing a large uncertainty, even for fresh fuel. In view of these challenges, more detailed simulation techniques have been adopted more recently, such as Potts kinetic Monte Carlo [348] or phase field modelling [349]. Their integration in fuel performance codes, however, remains challenging [231].

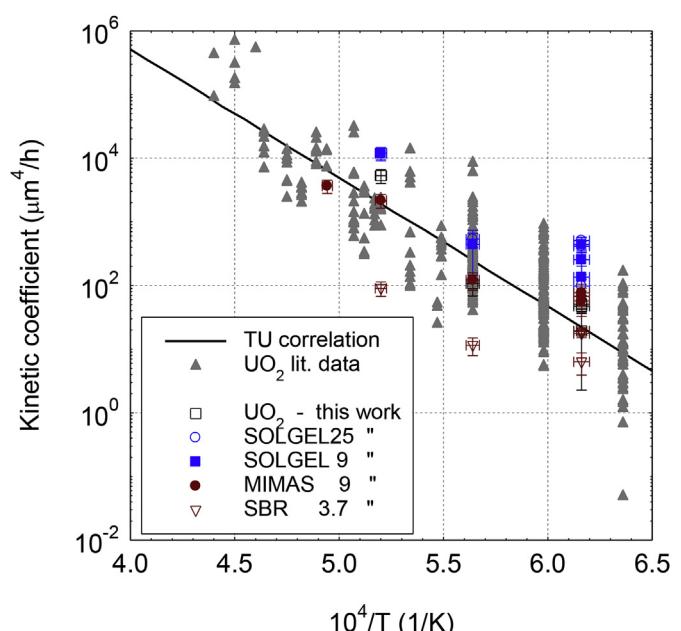


Fig. 14. Arrhenius plot of the kinetic coefficients for grain growth following expression the expression in Ref. [131].

4.3. Integral code validation and benchmarking

4.3.1. From post irradiation examination data to on-line measurements

Once all material properties and models have been validated separately with particular assumptions or under specific circumstances and combined in a fuel rod performance code, it is important to assess the integral performance of the tool. Before online measurements became available, only end-of-life measurements could be used from PIEs with information at one specific time only. Such data include fission gas release, helium inventory, and rod-free volume on the basis of rod puncturing, clad diameter changes by means of profilometry, clad oxide thickness measurements based on eddy current measurements, fuel density changes obtained from immersion, grain size measurements inferred from ceramography, fuel stack length changes derived from gamma scanning, or fuel rod length variations obtained from metrology. Such data are very useful but expensive and time consuming to obtain. This changed drastically thanks to through-life data that have become available by means of instrumented rods in test reactors.

Many online measurements in experimental reactors rely on linear variable differential transformers (LVDT), which are used to measure displacement. LVDTs operate on the principle of a transformer and are used for measuring axial deformation of the fuel stack or cladding, but also for internal gas pressure variations via (bellows) pressure transducers. The fuel stack extensometers provide information about the combined effects of fuel thermal expansion, densification, swelling, creep, etc. The cladding extensometers provide data about thermal expansion, irradiation growth and creep, but they can also provide information about the pellet-cladding mechanical interaction.

Each of the instruments provides a piece of information about one specific aspect (e.g. thermal or mechanical behavior) of the integral fuel rod behavior. More recently, however, several instruments have been combined in order to provide simultaneously and through-life information about different aspects of the fuel behavior that are interdependent [350]. As an example, simultaneous recording of the inner gas pressure along with a central thermocouple can provide valuable information about the temperature level, above which there can be an escalation in thermal fission gas release or the onset of cladding lift-off.

For the online assessment of radioactive fission gas release, or the hydraulic diameter measurements in order to assess the remaining gap width, gas flow lines have been attached to fuel rod segments in the Halden reactor (e.g. Ref. [351]). The same setup has been applied to assess diffusion coefficients for volatile fission products for instance by using sweep gases to carry released fission gases from the fuel rod to a detector situated outside the reactor. Such measurements complement the more commonly applied bellow pressure transducer, which relies on the LVDT, where online pressure variations can be directly compared with fission gas release predictions of the codes, for example to assess the onset temperature for release as a function of the burnup [352,353].

Based on the available experimental data and in accordance with the regulatory requirements for fuel licensing [354], the integral assessment of the fuel rod performance codes has typically focused on a few main areas [44,45,112,117,175,246,285,355–358]: thermal performance, fission gas release, pellet cladding mechanical interaction, cladding creep, growth, corrosion and hydrogen pickup. For the assessment of the fuel central temperatures, thermocouples or expansion thermometers are used (e.g. Ref. [359]), providing a substantial number of data points as measurements can be recorded every 15 min for months or years. Because the main thermal resistance in the fuel rod is that of the oxide fuel pellet in

addition to that in the fuel-to-pellet gap, such measurements can also provide insight about the gap size evolution (due to relocation, densification, etc.) at the beginning of irradiation, especially when both cladding corrosion and fission gas release can be neglected. A typical comparison of measured fuel centerline temperature to predictions from the Bison fuel performance code is shown in Fig. 15 [44]. Measurements are from four fuel rods instrumented with centerline expansion thermometers and irradiated in the Halden research reactor.

For normal operating conditions cladding diameter (creep down) and rod growth measurements are used for validation, mostly from post irradiation measurements, and (to some extent) from in-pile measurements in test reactors like Halden. Experimental data on mechanical interaction for PCI and PCMI have also been gathered in the IFPE database. They are subdivided into three broad categories [360]: fuel rod diameter changes caused by a period spent at higher-than-normal power in order to assess the hoop strain limit, the result of power ramp testing to define a failure threshold (e.g., versus burnup), and single effect studies to measure changes in gaseous porosity that cause fuel swelling during controlled test conditions.

Much of the assessment of clad corrosion and hydrogen pickup models for zircaloys relies on access to commercial data. Only codes developed by an industrial organization (e.g. PAD5, GALILEO, etc.) with a sufficiently large database and access to data for each rod and coolant conditions of the plant can make a detailed comparison for each alloy. The so-called generic codes like FRAPCON, FEMAXI and TRANSURANUS usually provide their user group with correlations compared against a large (undistinguishable) quantity (or cloud) of corrosion data versus burnup. Nevertheless, such data prove sufficient for a best-estimate analysis, since the deviations have a limited impact on fuel rod behavior for the licensed discharge burnup values. This is especially true with modern cladding materials with around 1% Nb for example that have outstanding corrosion resistance. Technical safety organizations making use of such generic codes have access to the confidential data and can implement the more accurate specific correlations of the industry.

4.3.2. The role of international benchmarks

The simplest way to obtain an overview of the current status of the various fuel performance codes and their validation has been

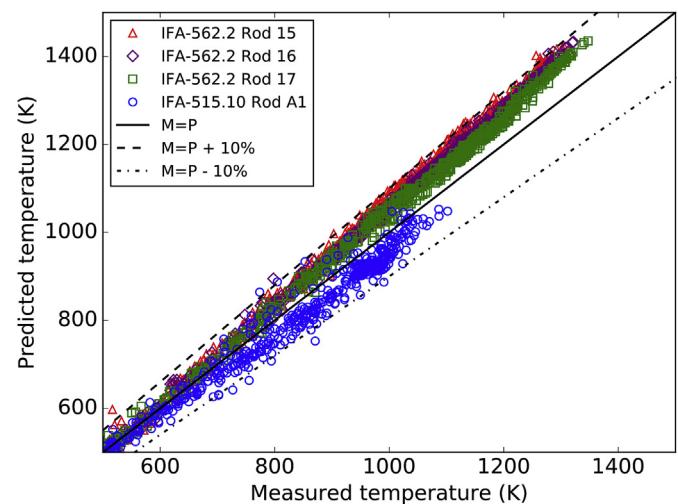


Fig. 15. Comparison of measured fuel centerline temperature to predicted values from the Bison fuel performance code [44]. Measurements are from four fuel rods irradiated in the Halden research reactor and cover a burnup range from zero to 60 MWd/kgUO₂. M = P stands for Measured = Predicted.

via international benchmarks such as those organized both by the IAEA and the NEA. They have also been instrumental in the development as well as in the validation process of some of the fuel performance codes, fostering international and bilateral cooperation as well.

The first benchmark organized by the IAEA in the mid-1980s was in the form of a project entitled "The Development of Computer Models for Fuel Element Behavior in Water Reactors" (D-COM) that involved 16 codes (e.g. Ref. [361]). The primary objective was the assessment of fuel performance code predictions for fission gas release. To this end, the participants were required to simulate three mini-rods with a maximum burnup of 32 MWd/kgHM. In a first step, blind predictions were compared with the experimental data [362]. On this occasion only a few codes correctly predicted that most of the gas release occurred during the bump test in two rods. In a second step, the percentages of gas released were recalculated by means of improved code versions [363].

The second benchmark organized by the IAEA took place from 1992 to 1996 [364]. It was a project called Fuel Modelling at Extended burnup (FUMEX), with 19 participating codes from 15 countries. In a similar way as for the D-COM exercise, the participants were first required to perform blind predictions. The cases involved 10 fuel rods with a burnup range up to 50 MWd/kgHM from 6 experiments and were provided by the OECD Halden Reactor Project. Nevertheless, the preliminary results were obtained without specific models for the HBWR conditions. The benchmark addressed not only the fuel thermal performance, but also fission gas release and to a limited extent pellet cladding mechanical interaction. The blind comparison revealed discrepancies in terms of temperatures, especially at high burnup. This stimulated the development of improved versions of the models for radial power prediction (e.g. TUBRNP) [108] and were implemented in both TRANSURANUS and FRAPCON [162]. Another improvement dealt with Xe depletion models for the HBS [365]. All the improvements lead to better predictions of gap conductance, center temperature and swelling, hence also the final results for fractional fission gas release predictions [366]. The mechanical behavior on the other hand was not analyzed in great detail.

Another major consequence of FUMEX was the establishment of the IFPE database [314]. Furthermore, a collaboration between Euratom and the IAEA enabled the TRANSURANUS code to be transferred to independent nuclear regulatory authorities being established in several Eastern European countries [364].

The third benchmark for LWR fuel behavior codes organized by the IAEA from 2002 until 2005 was FUMEX-II [170]. Its aim was to evaluate code thermal performance, fission gas release and pellet-cladding interaction for high burnup UO₂ fuel. A total of 27 cases were simulated. Some of them dealt with so-called "nominal" cases. These were specifically selected to test the capabilities of the codes at ultra-high burnup levels up to 100 MWd/kgHM with simplified irradiation histories. Because such discharge burnup is well beyond the range in commercial reactors, data are very scarce in the open literature. The majority of cases were already included in the IFPE database, while the others were introduced afterwards. Most of the cases were thus not unknown to the 19 participants.

Considering the large number of cases and project partners, the overall outcome of FUMEX-II was more complex:

- The so-called "user effect" had to be dealt with since a few codes were being used by several participants (e.g. TRANSURANUS users from Bulgaria, Germany, Romania and Switzerland [367]). Similar user effects were reported later [290] in the RIA benchmark organized by the NEA (see below).
- Satisfactory fission gas release predictions were reported during steady-state, confirming previous evaluations. Nevertheless, the

kinetics of burst release associated with sudden power variations such as a power drop, were typically not well reproduced. Moreover, a systematic but moderate under-prediction of gas release during ramp tests was reported. Improved predictions of integral fission gas release at high power were obtained following the inclusion of grain boundary sweeping as a result of grain growth or extended cracking in high burnup fuel during power ramps.

- Based on the nominal cases, it was also concluded that the codes were mature and able to deal properly with fuel behavior up to 100 GWd/tHM without numerical problems.
- More elaborate models for the HBS were launched and discussed. Some of them considered the dependence of the formation on the initial microstructure (e.g. grain size) or the capability for retaining fission gas, and experimental uncertainties were analyzed via a sensitivity analysis. In the meantime, new experimental observations indicated that the HBS porosity is not interconnected, and could therefore not explain the increased integral release fractions obtained by post irradiation examination of commercial rods [173]. Further progress in modelling the HBS was hindered by the limited amount of data in open literature and ongoing discussions about the formation mechanisms (the interested reader is referred to Ref. [73] for an extended recent overview).
- There was a need to extend the mechanical analysis, since no definite conclusions could be drawn from evaluating cladding deformation in two cases.
- Similarly, the behavior during loss-of-coolant accidents (LOCA) could not be properly evaluated based on too few simulations from the participants.

In the wake of the FUMEX-II project, several participants continued using the IFPE for developing a complementary component of fission gas release triggered in the event of rapid power variations (e.g. Ref. [34]).

The success of previous benchmarks and the remaining open questions triggered FUMEX-III (2008–2012) [368]. The 30 participants originally expressed a large range of interest, including on one hand all LWR types as well as CANDU, and on the other hand topics ranging from mixed oxide fuels and Gd-doped fuels to design basis accidents, pellet cladding (mechanical) interaction, etc. Accordingly, a test matrix was put together. For each topic and reactor type only a subgroup of interested participants was involved. These subgroups focused on a specific number of so-called priority cases. Despite the scattered activities, some general observation could be formulated.

- In particular, the predictions of fuel center temperatures for UO₂ during normal operating conditions up to burnup levels about 60 GWd/tHM are all in fair agreement. For MOX fuel, however, there remained some uncertainty about the extent of thermal conductivity degradation.
- Most codes consider some fission gas release from the HBS in order to be able to reproduce enhanced release measured in high burnup fuel, although there is no consensus about the detailed mechanisms partly caused by the limited resolution of the data.
- Only a few codes were able to match the failure criterion separating the non-failed from failed rods, although many upgraded their predictions after improving the fuel swelling model.
- The cladding deformation following normal operation or a ramp was satisfactory, and 3D modelling showed excellent results in terms of clad ridging.

- The idealized cases have been well appreciated in order to identify issues of common interest for further development (e.g. about HBS release), as well as the idea of applying sensitivity (and uncertainty) analysis.

Finally, too few simulations and data were available to draw conclusions about the DBA simulations.

In 2004, the working group on fuel safety (WGFS) of the OECD-NEA organized a code benchmark for fuel rod behavior under LOCA conditions [369], based on some Halden LOCA tests IFA-650.3-5. The benchmark was carried out in two steps. At first, only IFA-650.3 was pre-calculated by the codes. The outcome of the blind predictions revealed quite a bit of scatter in results, especially a conservative underestimation of the burst time. After corrections, and in particular using unified thermo-hydraulic boundary conditions, the burst time predictions matched the experimental observation much better, even though strain profiles showed severe over-estimations. This was largely caused by an anomaly in the failure at a weak spot due to the thermocouple welding, but it is in line with the observations in the more recent FUMAC benchmark (see below). In a second phase, the code predictions were compared with the results from the IFA-650.4 and 5 tests. The analysis which ended in 2010 revealed that the clad temperature plays a predominant role and that code improvements based on axial relocation models were crucial to model the relocation phenomenon during LOCA in high burnup fuel (e.g. in IFA-650.4) and to calculate the consequences on local cladding oxidation and concomitant embrittlement. The recommendations have been implemented by some of the participants of the FUMAC benchmark of the IAEA.

Shortly after the LOCA benchmark, the WGFS organized a similar code benchmark for fuel under another design basis accident, namely the reactivity initiated accident. In the first phase (2010–2013) [265], the 17 participating organizations simulated 4 RIA experiments: 2 tests performed in the NSSR in Japan and 2 tests in the CABRI reactor in France. Emphasis was on evaluating modelling options for fuel rod codes in terms of reproducing experimental results as well as extrapolating to typical reactor conditions. The outcome was encouraging, but a lot of scatter in the results (especially in cladding temperatures when boiling occurred) led to the definition of a second phase of the benchmark that was launched in 2014 [290]. The focus of the 15 participants was on understanding the differences in modelling based on simplified cases and on applying uncertainty and sensitivity analysis. The third phase of the benchmark was launched in 2018. Its objective is to complete the second phase with irradiated fuel by performing a similar uncertainty and sensitivity analysis.

In the wake of the nuclear accident in Fukushima, the IAEA organized a coordinated research project FUEL Modelling under Accident Conditions (FUMAC) between 2014 and 2018. Although the general objective was to better understand the fuel behavior in accident situations, the 27 participating organizations focused on loss of coolant type accidents, while attention was also given to the severe accidents as well as accident tolerant fuels, albeit to a lesser extent. The experimental data selected included separate-effect tests on cladding material from Hungary, out of pile clad bundle tests from Germany, out of pile single rods tests with irradiated fuel from Sweden and in pile single rod tests with both PWR and VVER irradiated fuel rods from the Halden Reactor Project, as well as severe-accident tests with bundles from Germany. Whereas the first phase of the project was dedicated to some model developments and the simulation of the individual experiments, the second phase of the project involved the application of common hydraulic boundary conditions in some tests as well as the uncertainty and sensitivity analysis. The results are being prepared for

publication [268,370].

Following the launching of the benchmarks for design basis accident conditions by the NEA and IAEA, and the limited attention for the phenomenon the NEA launched one specifically dealing with the PC(M)I issue in 2015 with 18 participants [371]. Four hypothetical cases were selected to start with. The preliminary results pointed out that even for fuel stack elongation, clad elongation, clad outer diameter and clad hoop stress versus time, for which the evolution is similar for all codes involved, there are surprising differences at time zero. These preliminary results were discussed along with code capabilities to analyze PC(M)I at the workshop “Pellet-Clad Interaction (PCI) in Water-Cooled Reactors” sponsored by the NEA Working Group on Fuel Safety (WGFS) and held in Lucca, Italy [372]. With regards to modelling and simulation, key conclusions from the workshop include:

- Despite concerted efforts to model the large PCI experimental database, it is apparent that existing PCI models are not able to distinguish failure from non-failure. This is likely because the existing PCI experimental database is extremely heterogeneous and because of the stochastic nature of some phenomena involved.
- Conventional 1.5D and new 3D codes remain complementary, with the 1.5D codes still forming the basis of industrial applications. It remains difficult to explain why some rods do not fail under power transients or why some pellet types exhibit higher PCI resistance with respect to standard fuel. Multi-dimensional modelling is needed to understand PCI failures because these occur at pellet interfaces, where local deformations develop that are not reproduced by 1.5D codes.
- Further progress will require the definition of a PCI failure criterion. PCMI must be evaluated before PCI, and several parameters that can be model-dependent are candidates (e.g., stress, strain, strain energy density, damage parameter) although some cannot be measured directly.

These conclusions are in line with those from the recent review of the PCI subject by Piro et al. [373]. After completion of the NEA benchmark on PC(M)I foreseen in 2018, a second, follow-on PCMI benchmark exercise is being considered that would look at the effects of uncertainties.

5. Concluding remarks

Nuclear fuel rod performance codes have been developed worldwide for about 60 years for design optimization, experiment planning and interpretation, and safety analysis. Some of the simulation tools are developed and applied by industry, and hence are not publicly available, whereas others are developed and used by research centers, universities (in part for training purposes) and safety organizations. Most of them have achieved an acceptable level of maturity, which is in line with the very low failure rates observed in commercial nuclear power plants today. The current level of maturity is reflected in the latest international code benchmarks organized by the IAEA and the OECD-NEA.

The progress is largely based on the improvement of our understanding about the myriad of phenomena observed in the rods, as well as their corresponding equations, and the accumulation of material properties via increasingly detailed experimental data, be it via out-of-pile or in-pile measurements. The acquisition, assessment and organization of experimental information in common databases (e.g., IFPE) as well as libraries (e.g., MATPRO) have largely contributed to knowledge preservation and decent quality standards. Similarly, the creation of large user groups for some of the fuel performance codes have enabled increasing common

developments, but also contributed to their independent verification and validation that is necessary for quality assurance purposes.

Over the past decade a certain number of developments have contributed to new opportunities. They include hardware and software developments, thanks to which multi-scale and multi-physics simulations have received renewed interest. Also uncertainty and sensitivity analysis is being systematically applied for fuel performance simulations. Finally, international benchmarks have enabled dissemination of knowledge gained and improvement of code models.

On the basis of the outcomes of the various benchmarks and separate validation efforts reported in the open literature, there are still a number of outstanding challenges for the research community:

- Some data remain insufficient, especially with respect to the new materials (e.g. EATF).
- New operating conditions (increased discharge burnup, changing electricity markets, etc.) require updating of some safety criteria (e.g. account for hydrogen content in LOCA safety criteria).
- The validation of fuel performance codes for design basis accidents is encouraging but not at the same level as that achieved for normal operating conditions, especially for fuel employing new materials.
- The large amount of experimental data generated and the increased level of complexity of the simulation tools requires a certain level of reduction or condensation of the data, despite the available computational resources.
- The coupling of different modelling tools for multi-physics simulations poses new challenges in terms of verification and validation methods, as well as new validation data.
- The increased number of users for one particular code sometimes brings about confusion in terms of version used, in addition to the so-called user effect. At the same time, it offers great opportunities for synergies of resources for common developments as well as an independent validation.
- There is a need to make better use of uncertainty and sensitivity analysis, which becomes available thanks to statistical tools, but for which there are still many open questions as revealed during the BEPU conference in 2018.

The common code developments enabled by the user groups, along with international benchmarking, should enable fuel performance modelling to cope with these challenges.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jnucmat.2018.12.037>.

Appendix. Overview of main fuel rod performance code developments across the globe

In Europe, many different codes have been developed. Since 1967 the COMETHE code [374–376] has been developed in Belgium by Belgonucleaire. The code was originally developed for fast breeder reactor fuels, then for UO₂ and especially MOX fuel simulations during normal operation conditions in LWRs [138,377,378].

More recently, after the restructuring of the Belgian industry and the ensuing end of the COMETHE developments, the efforts of the Belgian National Nuclear Research Center SCK-CEN turned to the MACROS code [115], which was developed based on the Russian ASFAD code [379]. This code is used for research purposes and can deal with a variety of oxide fuel materials (including U, Th, Pu and others) and flux spectra (FBR and LWR).

In the Czech Republic, the PIN code [380] has been under development since 1982 at the national nuclear research center (UJV) on the basis of the GAPCON-THERMAL2 code, which was developed in the USA for fuel under steady state conditions. On the basis of their own specific data, as well as those published by Strijov et al., researchers in the Czech Republic improved the material properties for VVER-440 and VVER-1000 fuel in the PIN-micro code in 1988 [381].

In France, the COPERNIC and CYRANO codes were developed by Framatome and EdF respectively. The COPERNIC code [175] was derived from the TRANSURANUS code [193] developed in Germany, as outlined below. Although EdF acquired the TRANSURANUS code at the beginning of the 1990s and used it in the IAEA benchmark FUMEX [382], the CYRANO3 code [383] is the second-generation code from EdF. It was developed toward the end of 1998 to perform all the design calculations for UO₂ with or without additives and MOX fuel. The SCANAIR code [384] was developed by IRSN for specific reactivity initiated accident conditions and is currently distributed to a number of EU organizations. The CEA has developed different codes [120]. The METEOR-TRANSURANUS code [385] was developed for PWR fuel, along with specific finite-element-based tools for multi-dimensional analysis, such as the TOUTATIS code for PCI analysis. All these code developments have been integrated in the PLEIADES platform, which was co-developed by the CEA, EdF and Framatome. The CYRANO3 code has also been integrated into PLEIADES [383]. The PWR application has become ALCYONE, which provides a reference simulation tool in a so-called one-and-a-half dimension (1.5D), along with the two-dimensional (2D) and three-dimensional (3D) local analysis tools for specific studies such as PCI. It is dedicated to in-reactor behavior of UO₂-based or MOX fuel during both normal and off normal operation conditions.

In Germany, the CARO code was developed by Siemens [160] for normal operating conditions of UO₂ and MOX fuel. Nevertheless, the common tool GALILEO, developed by the global Framatome company, has been created more recently on the basis of the CARO-E3, COPERNIC2 and RODEX4 codes [117]. The RODEX code was developed in the USA for BWR fuel types.

The URANUS code [61,386,387] was subsequently developed at the technical University of Darmstadt and the national nuclear research center in Karlsruhe (KIT, formerly KfK and FZK). It was initially developed for a variety of fuels, cladding, and coolants for fast reactors under both normal operation as well as accident conditions. Since the later 1980s, however, the focus of developments has turned to LWR fuel at the JRC of the European Commission, and the code has been renamed to TRANSURANUS [109]. With the support of the IAEA following the FUMEX code benchmark, the JRC distributed the TRANSURANUS code to many organizations in new EU member states operating the Russian-type VVERs. With the support of the user network, which includes more than 40 organizations world-wide, the code was further developed for design basis accident conditions, such as a loss of coolant accident (LOCA), and is used in licensing by both industry and nuclear safety authorities. For such simulations, as well as for modelling of storage conditions, the code requires, upon input, boundary conditions for the coolant, such as temperature, pressure, and heat transfer coefficient. These are typically obtained from system codes like RELAP or ATHLET. In order to facilitate such data transfer,

various code coupling developments are underway. This includes its integration in the EU NURESIM platform, which is based on the SALOME open-source platform developed by CEA, EdF, and OPENCASCADE.

Finally, the technical safety organization GRS developed a specific simulation tool TESPA for the analysis of fuel cladding under LOCA conditions in the early 1980s [264]. More recently this simulation tool has been extended to the TESPA-ROD tool [388], which enables simulation of a full rod in 1.5 D under DBA, normal, and storage conditions.

Over the last decade, the center for energy research from the Hungarian academy of sciences (MTA EK), has developed the FUROM code [45] for the simulation of the Russian-type VVER, as well as the PWR UO₂ fuel with the corresponding cladding materials E110 and Zry4 respectively. The code was based on considerations from the PIN Micro code [380,389–391] from the Czech Republic for VVER fuel. It is used for normal operation conditions as well as anticipated operational occurrences in the VVER-440 fuel licensing of the fuel for the Paks NPP.

In Sweden, ABB Atom developed the STAV code [392] based on finite element analysis for the simulation of BWR and PWR fuel under steady-state conditions and operational transients. Westinghouse Electric Sweden further developed the STAV-T code [393] for accident analysis such as LOCA, providing both an axisymmetric analysis first with a limited number of axial segments, followed by a local 2D plane model analysis at the peak power axial position.

In the UK many codes have been developed over the past five decades. The chronological evolution was summarized by Matthews in 1986 [394] and, more recently, in 1990 after 25 years of development [395]. Today, only the ENIGMA code is used for LWR applications. This is the result of a combined effort among industry and research organizations that originally worked on separate tools such as Minipat, Sleuth and Hotrod. Starting in 1986, ENIGMA's early development was done by the UK fuel vendor and utility at the time—British Nuclear Fuels plc (BNFL) and the Central Electricity Generating Board (CEGB), respectively [266]. The code is currently being developed by National Nuclear Laboratory (NNL; formerly the R&D division of BNFL), EDF Energy (formerly CEGB) and VTT (a Finnish research organization) [266,396]. ENIGMA is used for fuel licensing in the UK's AGRs and PWR (Sizewell B) and for research purposes. It has also been used for licensing of fuel in overseas reactors (the Loviisa VVER-440 and the Beznau PWR) for which BNFL supplied fuel.

In China, several codes have been under development more recently. The FROBA code has been developed at the Xi'an Jiaotong University specifically for the application to the AP1000 reactor [397]. The FUPAC code [398] was developed by NPIC for normal operations of PWR fuel rod but with special models for N36 cladding [399,400], which is a new zircaloy also developed by NPIC. CIAE developed the FTPAC code [401] for transient and accident conditions, while the JASMINE code [402,403] was developed by CGNPC and integrated into the FEPAC platform for fuel assembly performance analysis.

The COSMOS fuel rod performance code [136,404] has been under development in South Korea by KAERI since 1996 for the simulation of conventional UO₂ with a focus on MOX fuels during both steady-state and transient conditions in LWRs. In parallel, the INFRA (Integrated Fuel Rod Analysis) code [167,168] has also been developed for the analysis of high-burnup UO₂ fuel, which also includes a coupling to a finite element model for PCMI. The main purpose of the COSMOS code is to calculate the temperature distribution in the fuel and cladding, as well as fission gas release from the fuel. Further developments of COSMOS include the capability to deal with re-fabricated and instrumented rods in experimental reactors and the high-burnup issues, such as the HBS development

(see details in specific review [73]), as well as clad corrosion and creep [112]. More details can be found in the recent review of the fuel technology developments in Korea by Koo et al. [405].

In Japan, the integrated fuel performance code FEMAXI has been under development since 1974 by JAEA (formerly JAERI). The first version mainly aimed to analyze pellet-cladding mechanical interaction (PCMI) in a fuel rod under in pile conditions. The second version [406], developed in 1977, included an elastoplastic-creep stress-strain analysis of relaxation. The third version [407] was developed under an extensive cooperation among JAERI, Sophia University, NFD, CRIEPI, and CRC. Subsequent versions of the code have been developed by JAEA in order to deal with more elaborate thermal and mechanical analysis, transient conditions [408–414], high-burnup fuel behavior analysis [166,415], and MOX fuel [186,416]. Most recently, the seventh version [256] also covers more mechanistic fission gas behavior and the restart option following a base-irradiation. In parallel with and on the basis of the development of FEMAXI-7, RANNS has been developed by JAEA for the thermo-mechanical analysis of a single fuel rod mainly under reactivity-initiated accident (RIA) conditions [417,418]. The RANNS code has been developed in order to understand dynamics that may lead to rod failure and also to predict fuel rod failure under RIAs. More recently, the implementation of some functions has been completed for calculating the fuel rod behavior in loss-of-coolant accident (LOCA) conditions [419] as well. The improvement of both FEMAXI and RANNS still continues, and the codes are to be integrated into one in the future.

Other fuel performance codes were developed in Japan by industry entities in the 1980s and have been reviewed by Kinoshita in 1993 [420]. They include the TRUST code, developed by NFD and used in FUMEX [382]; the EIMUS code, developed by CRIEPI for high-burnup analysis; and the IRON code, developed by Shikoku Electric Power Company for analysis of fuel reliability during load following transients. Both EIMUS and IRON were derived from FEMAXI-III.

In the rest of Asia, the development of codes is less well-documented and is evolving. In India, fuel performance codes for LWR fuel have been developed by the National Research Center (BARC) and the Nuclear Power Corporation (NPC). More precisely, the PROFESS code was developed by Sah et al. [421] in the early 1980s for the interpretation of post-irradiation examination results of zircaloy-2 cladded UO₂ and MOX fuel rods irradiated in either BWRs or PHWRs. It has been applied in different code benchmarks (e.g., D-COM and FUMEX-II) organized by the IAEA (see Integral code validation and benchmarking) [157,382]. In parallel, Prasad et al. [382] developed the FAIR code bases on finite element modelling in two dimensions for PHWR fuel, but also took part in FUMEX-II for LWR simulations although the code is validated for low burnups (5 GWd/tHM). Starting in the 1970s, the FUDA code was developed by Das et al. [157,382] of PNC. This was developed essentially for PHWR fuel but could also be applied to LWR fuel in the frame of FUMEX and FUMEX-II.

In Russia, the main simulation tools currently used by the industry for nuclear fuel simulation are START-3 [158,159,422,423] for stationary conditions and RAPTA5.2 for accident conditions [424–426], both developed by the All-Russian Scientific Research Institute for Inorganic Materials (VNIINM) starting in the 1970s [427]. The fifth version of the RAPTA code is comprised of new models, such as the non-axisymmetric local ballooning of cladding, and mutual effects within a fuel bundle for cladding straining. During and after completion of FUMEX-I in the middle of the 1990s, a serious upgrade of the START-3 code was also undertaken for simulating high-burnup fuel under normal operation conditions. The RAPTA code is used for simulation of water-cooled fuel (VVER, LWR, RBMK) under accident conditions like LOCA and RIA. It uses

input data from START3 in a manner similar to FRAPTRAN's use of data from FRAPCON (see below).

More recently, two other codes have been developed by research organizations in Russia. The SFPR code [84,86] has been developed by IBRAE in 2011 on the basis of the MFPR code for fission product behavior [87] and the SVECHA/QUENCH code developed for severe accident simulations in the 1990s in collaboration with different European organizations [428]. The MFPR code was developed by IBRAE in collaboration with IRSN (France), although both organizations developed their own versions since 2011. The RTOP code [429] has been developed by TRINITI at the end of the 1990s on the basis of a mechanistic model for the kinetics of UO_2 oxidation in steam, grain growth [133] and fission product behavior [430]. At the beginning it aimed at modelling of defective fuel behavior and fission products propagation in the primary circuit of water-cooled reactors. More recently, the code has been extended to simulate both normal operation as well as accident conditions [429,431], making use of a local 3D analysis tool in addition to the conventional 1.5D analysis [432].

In the United States, development of the FRAP series of codes for conventional oxide fuels began in the late 1970s, evolving as a joint effort between Idaho National Laboratory (INL) and Pacific Northwest National Laboratory (PNNL). Using 1.5D geometry, FRAPCON [66] considers normal reactor operation while FRAPTRAN [67] simulates accident behavior. Both codes were developed for the U.S. Nuclear Regulatory Commission (NRC) to support regulatory analysis. FRAPCON and FRAPTRAN were recently merged to form the NRC's new fuel performance code FAST [259].

On the side of the utilities, the Electric Power Research Institute (EPRI) originally supported two fuel performance codes: ESCORE for steady-state reload analysis and FREY for fuel reliability and off-normal transient analysis. However, in 1996, EPRI initiated development of the FALCON code [68,69,248] with the Anatech company, combining the best features of ESCORE and FREY. This combination is applicable to both normal operation conditions as well as design basis accidents. FALCON is finite element-based and can be used for 2D analysis with either axisymmetric or Cartesian geometry.

Since 2009, INL has been developing a modern finite-element-based nuclear fuel performance code known as BISON [243]. As applied to LWR fuel, BISON supports the use of a variety of geometries (1.5 and 2D axisymmetric, 2D Cartesian, or 3D) all with the same material and behavioral models. BISON supports parallel computation and employs a software architecture that minimizes the programming required to add new features, such as material and behavior models. In recent years, capability has been added to BISON to support accident analysis (LOCA and RIA) [263].

Additional fuel performance codes have also been developed by industry, e.g. PAD5 (Westinghouse) [285], and RODEX (Framatome) which was later integrated in the GALILEO code [117].

In South America, specifically in Argentina, the BACO code [433,434] has been developed by the Argentine Atomic Energy Commission (CNEA). BACO has been under development since 1980 and addresses Pressurized Heavy Water Reactor (PHWR) and CANDU fuel. The CARO-D code was provided by KWU-SIEMENS from Germany in the 1980s to evaluate the Atucha-type fuel rod (PHWR) behavior under normal operating conditions. Since the FUMEX fuel rod code benchmarks organized by the IAEA in the 1990s, the BACO's capabilities have been upgraded to deal with PWR and MOX fuel for PWR, as well as UO_2 for BWR, and VVER fuel types [435]. The modular structure of BACO is compatible with different material properties for all components of the fuel rods, hence in the past few years, also properties for SiC and FeCrAl for the cladding and USi and UN for the fuel have been included [436]. In parallel to BACO, the fuel performance code DIONISIO, Version

1.0, was designed in the wake of FUMEX to describe the interaction between fission gas release and PCMI by means of finite element method in two dimensions [437,438]. A new version of the code, DIONISIO 2.0, has been recently developed [357]. The new code architecture allows the user to take into account the axial variation of the linear power and coolant temperature and, consequently, evaluate the dependence of all the significant rod parameters with the longitudinal coordinate. Some models to describe severe accident conditions were also introduced [439] in the timeframe of the last fuel code benchmark FUMAC organized by the IAEA.

Since 2011, the TRANSURANUS code has been acquired and adapted by nuclear power plant operator NASA for the safety analysis and optimization design for the Atucha II reactor, a PHWR constructed recently in Argentina and designed by Siemens KWU.

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