Main Concepts and Objectives of Fuel Performance Modelling and Code Development

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1 Introduction

Since the commissioning of the first commercial nuclear power station at Shippingport, 35 years of development have been spent improving the reliability, operating flexibility, safety and economics of fuel elements. Reliable performance requires that the fuel behaves in accordance with stringent nuclear, thermo-hydraulic and mechanical design specifications. The very low current failure rates of approximately 0 to 0.005% prove that, from fabrication to discharge of fuel elements, the complex problems including the material behaviour during irradiation are well understood.

Besides reliability strong economical arguments justify further research and development: the annual fabrication costs of fuel assemblies for all reactors world-wide represent approximately 10 - 20 billion dollars per year.

The present status of Light Water Reactor (LWR) fuel element performance was presented at an international topical meeting ealier this year [1], a summary is given in [2]. Key issues are advanced zirconium alloys together with improved fuel element designs with the goal to further improve load following and to enhance the burnup. In addition, many specific questions such as the behaviour of MOX fuel, Gadolinium fuel, or the managing of failed fuel rods were discussed.

The detailed understanding of complex fuel rod behaviour could only be achieved by large irradiation programs such as the Halden, Studsvik, Riso and many other projects and by detailed modelling. In most cases only macroscopic quantities (such as temperature, fission gas release etc.) are measured and these are the result of the interplay between many complex micro/macro processes in the fuel (diffusion, cracking, bubble formation etc.). Therefore only theoretical models which take into account these complex processes can be used to adequately treat the tremendous amount of experience and experimental evidence available. We cannot review or even mention the many publications on fuel rod modelling and must refer to an international conference organized by IAEA [3] which gives the present status.

Theoretical fuel rod modelling has made a major contribution to the successful evolution of fuel rod design. Whereas up to the late seventies reactor operation was supported only by rather simple calculations, the situation has changed drastically. Safety requirements, considerations towards minimising the nuclear waste and economics require detailed analysis of fuel performance under normal, off-normal and accident conditions. In fact, there is a clear trend in increasing the number and size of fuel rod modelling groups in research, by manufacturers and licensing authorities. Thus it seems to be worthwhile to review the basic concepts of fuel rod modelling and discuss their limitations.

2 What Has to Be Modelled?

The macroscopic behaviour of a fuel rod is to a large extent determined by microscopic processes. Theoretical models should therefore include the relevant local phenomena but should of course also be able to predict macroscopic consequences such as radial and axial deformations of the cladding, cladding corrosion, cladding failure, pressure build-up by fission gas release etc. Figs.1 and 2 give two typical examples for macroscopic results taken from References [4] and [5]. The large scatter is due to different loadings and designs. It is expected from modelling that these differences are explained.

The following three figures show examples of fuel microstructures imaged by Transmission Electron Microscopy for LWR fuel rods which have been subjected to different irradiation conditions, and demonstrate the dependence of the macroscopic fuel behaviour on the local UO_2 microstructure.

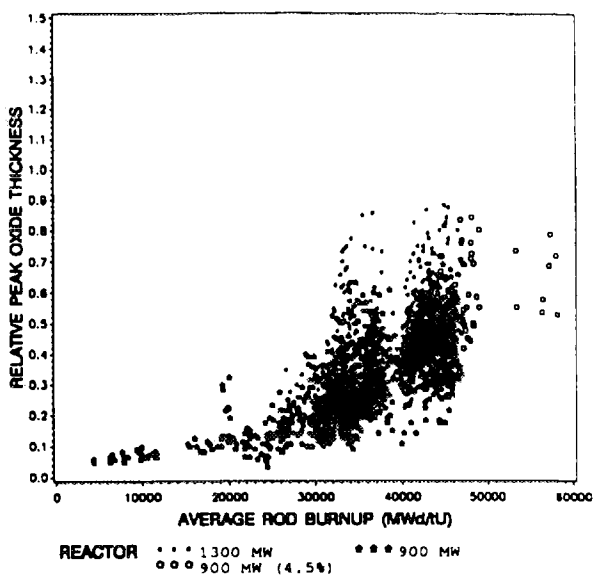

Figure 1 Relative peak oxide thickness as a function of average rod burnup according to Ref. [3]

Fig. 3 is an example of the fuel structure at the rim of a high burn up LWR fuel irradiated under steady state conditions to an average burn up of 75 *GWd/tM*, but with a local burn up at the fuel rim of about 200 *GWd/tM*. The original pre-irradiation fuel structure of large UO_2 grains with a typical grain size of 10 μm is seen to have restructured into very much smaller subgrains, typically 0.2 μm in diameter, separated by low angle grain boundaries - an example of one of the microstructural changes associated with the so-called "Rim Effect". The subgrains are free of dislocations and fission product precipitation. This transformation into a fine scale subgrain structure plays an important role in the local fission product release from the fuel.

Under steady state irradiation conditions at relatively low burn up most of the fission products remain in solid solution within the fuel matrix, or are contained in very small bubbles (< 10 *nm* diameter) or precipitates which can be redissolved by interaction with fission spikes. However, if the rating is increased above the steady state level higher fuel temperatures can lead to extensive redistribution of the fission products which can migrate rapidly to form bubbles and precipitates. Examples of such effects are demonstrated in Figs. 4 and 5 which are micrographs taken on LWR fuel samples which had been transient tested to a 25% increase in linear power for 24 *hrs.*, following steady state irradiation to a burn-up of approximately 4.5% FIMA.

In Fig. 4 large fission gas bubbles with diameters of 200 *nm* are found to have nucleated and grown on an extensive dislocation network, which serves as a rapid diffusion path for the fission gas in the fuel matrix. The formation of such bubbles leads to local swelling of the fuel (in this case about 4%) which can lead to very significant macroscopic effects when integrated over the fuel cross section. In addition the formation of fission gas porosity within the fuel matrix influences the local fuel conductivity.

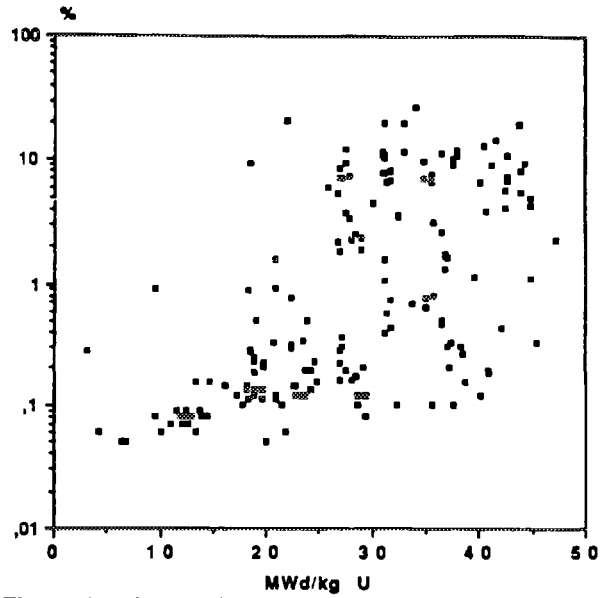

Figure 2 **Integral fission gas release for BWR rods according to Ref. [4]**

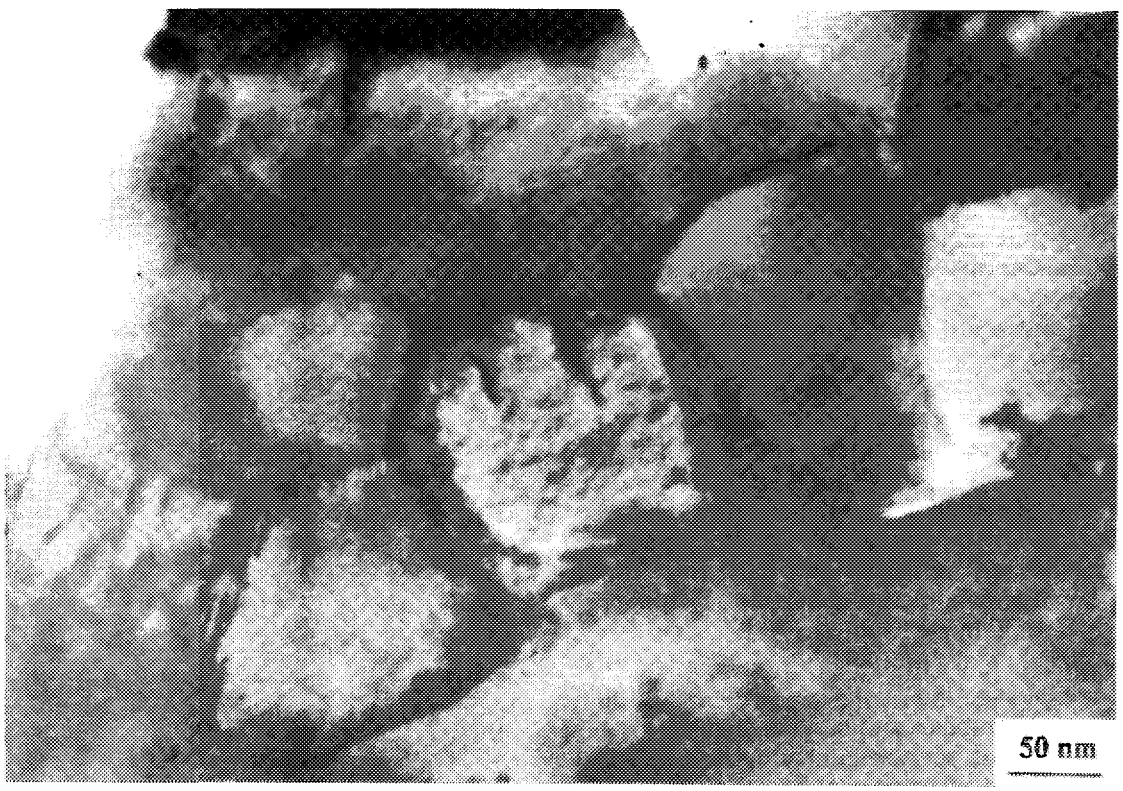

Figure 3 **Transmission Electron Micrograph of the rim of a high burn up LWR fuel sample, showing the restructuring into a fine scale subgrain structure, free of dislocations or fission product precipitation**

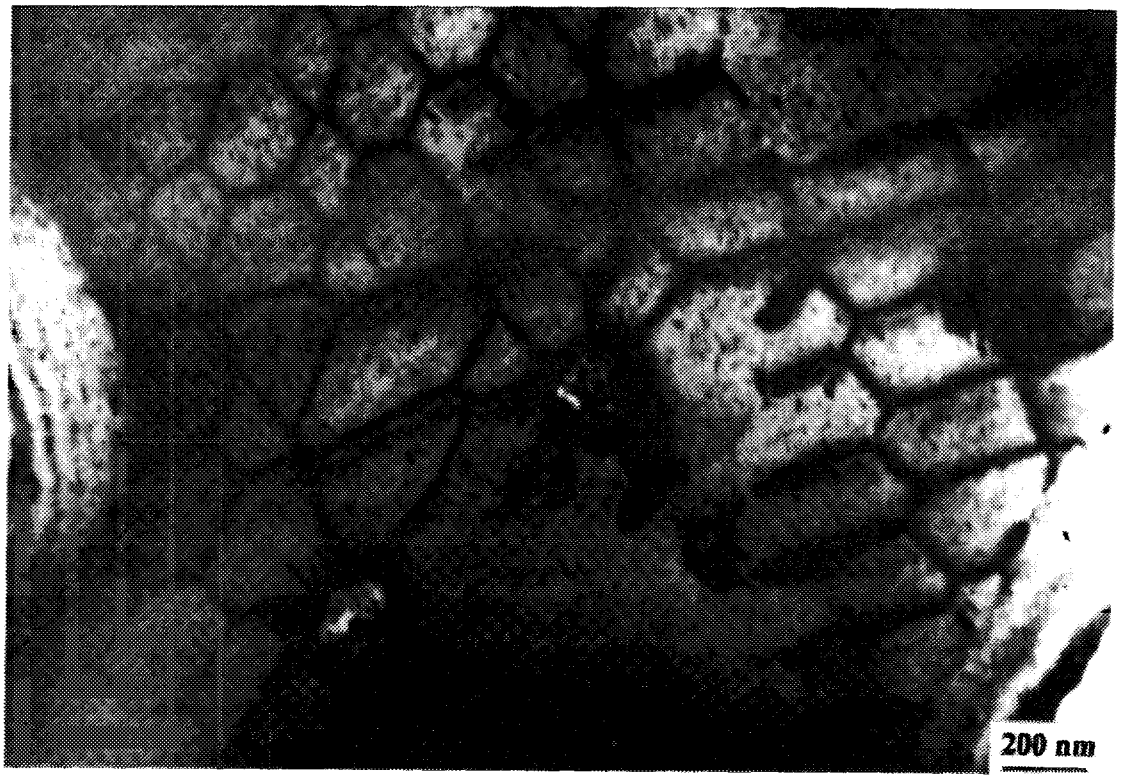

Figure 4 **Transmission Electron Micrograph of a transient tested LWR fuel sample showing the growth of large fission gas bubbles on a dislocation network within the UO_2 matrix**

A similar effect is demonstrated for the solid fission products in Fig. 5, taken on an LWR fuel sample with a similar transient history. A very large precipitate of the metallic fission products (Pd, Mo, Tc, Ru, Rh - a so-called 5-Metal particle identified by Energy Dispersive X-ray Analysis in the electron microscope) has grown within the fuel matrix, associated with extensive finer precipitation along the dislocation lines. The formation of such solid state precipitates also leads to fuel swelling, and, in addition, has important consequences for the distribution of released fission products following a reactor accident.

Figure 5 **Transmission Electron Micrograph of a transient tested LWR fuel sample showing the growth of a very large precipitate of the metallic fission products within the fuel matrix**

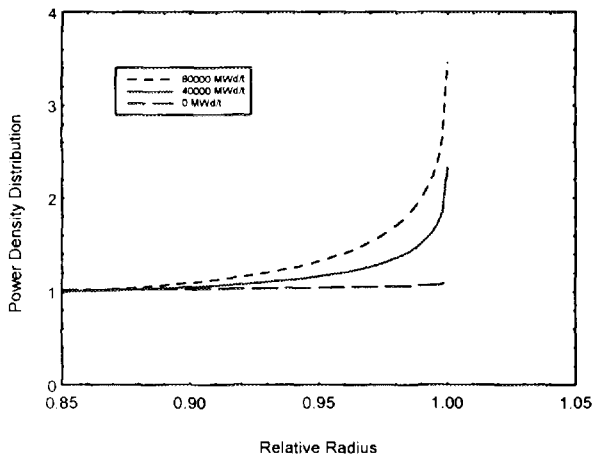

Figure 6 Radial power density distribution as a function of the relative fuel radius

These examples indicate just a few of the microscopic processes occurring at a local level within the fuel matrix which can have a determining influence on the macroscopic behaviour of a fuel pin.

3 Basic Equations

As already indicated, the fuel rod behaviour is determined by thermal, mechanical and physical processes such as densification, swelling, gas release, irradiation damage etc. Most of the physical processes depend exponentially on temperature and are highly non-linear functions of stress. Any fuel rod model must therefore include the solution of the heat conduction equation and the principal mechanical equations, i.e. equilibrium and compatibility, together with constitutive equations. These equations form the theoretical structure into which physical models must be incorporated.

3.1 Basic Equations of Heat Transfer

The calculation of temperatures in a fuel rod is one of the primary goals of fuel element modelling. The accuracy of these calculations influences such strongly temperature-dependent physical phenomena as fission gas diffusion and release, restructuring creep, thermal expansion, etc. In the following the uncertainties of the thermal analysis are outlined.

The basic principle of energy conservation must be applied and the thermal analysis in a fuel rod is governed by the heat conduction equation

$$c\,\rho\,\frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T + q''' \qquad (1)$$

where: c = specific heat, ρ = density,
T = temperature, λ = thermal conductivity,
q''' = power density.

As can be seen, the local temperature T depends on local material properties (thermal conductivity λ, specific heat c, density ρ) and the local power density q'''. In some models the radial distribution of the power density q''' is neglected. However, Fig. 6 clearly demonstrates that at high burnup this simplifying assumption is no longer valid. The temperature T also depends on time dependent boundary conditions and heat transfer coefficients (coolant-to-fuel rod and gap conductance).

Due to the numerous nonlinearities involved, only numerical techniques are possible which are of crucial importance because they determine the numerical reliability (stability) and to a large extent the total computer cost. Standard techniques such as finite difference or finite element are used and need not be discussed here.

It is pointless to ask what has the largest influence on the temperature distribution in a fuel rod for all real or postulated conditions. Nevertheless, under steady-state normal operation the gap conductance and the thermal conductivity λ dominate. However, this does not imply that the specific heat c and density ρ are of minor relevance. Since in most cases the thermal conductivity is only indirectly obtained from measurements of diffusivity, these two properties are of equal importance.

3.1.1 Thermal conductivity of LWR fuel

The thermal conductivity of LWR fuel has been extensively investigated, both theoretically and experimentally. A pioneering work on UO_2 is that of H.E.Schmidt [6] and the theoretical understanding is summarized by Hyland [7]. Three contributions are identified: conduction through lattice vibrations (phononic term), conduction through free electrons and a small contribution due to radiation. It is generally accepted that at lower temperatures the phononic term (2) dominates.

$$\lambda_{\text{phonon}} = \frac{1}{a + bT} \qquad (2)$$

The introduction of solid fission products and the formation of fission gas bubbles should decrease the thermal conductivity λ. Since point defects (oxygen interstitials or vacancies) and fission products act as phonon scatterers an extended phononic term of the form

$$\lambda_{\text{phonon}} = \frac{1}{a + a_x x + a_{\text{bu}} bu + bT} \qquad (2a)$$

seems to be justified, where $a_x x$ accounts for the effect of hypo- or hyperstoichiometry and $a_{\text{bu}} bu$ for the burn-up effect. The variable x is the stoichiometric deviation $|O/M - 2|$.

Today we have clear evidence for the degradation of the thermal conductivity λ with burn-up from three sources:

1. Fuel centre line temperature measurements performed at Risoe on refabricated fuel rods with different designs and burn-up levels [8].
2. Fuel centre line temperature measurements performed at Halden on specifically designed fuel rods with a small pellet-to-clad gap, negligible fission gas release and fuel restructuring proved the degradation of λ with burn-up. A reduction of 6 - 8% per 10 *Mwd/kg* UO_2 was found by Kolstad and Vitanza [9].

3. Measurements performed on SIMFUEL (SIMulated high burn-up nuclear FUEL) with an equivalent burn-up of 3 and 8 atom% provided data of the intrinsic conductivity (i.e. without gas bubbles, cracks etc.) and proved a degradation of the thermal conductivity λ with burn-up. The reduction was approximately linear with burn-up, Lucuta et al. [10].

Direct centre line temperature measurements on irradiated fuel rods give only an integral information over the entire fuel rod, whereas the measurements performed on SIMFUEL give local values.

All findings are in agreement with what is expected from theory. It can be concluded from the general Eq. (2a) that the degradation of the thermal conductivity λ with burn-up is more pronounced at lower temperatures. Kolstad and Vitanza obtain the factor $a_{bu} >> 0.014 - 0.016$ *mK/W* per atom percent burnup, Lucuta et al. obtain almost the same factor although their correlation is more complicated.

Apart from the temperature, the thermal conductivity of UO_2 also depends on the porosity P, the oxygen-to-metal ratio O/M (stoichiometry) and the burn-up bu. These relations are known for nearly 20 years [11].

Porosity in a ceramic material invariably decreases the thermal conductivity. Geometry (morphology, size, shape, orientation) and physical properties (emissivity of the solid, properties of the gas trapped inside the pores) are of importance. Theoretically, all of these effects are in principle understood. The problem, however, is the determination of the detailed relations. At the beginning of irradiation a given fabrication porosity (pores with a given size distribution and morphology) exists, which decreases during irradiation. Simultaneously, depending on irradiation conditions, new classes of porosity evolve, mainly at grain boundaries but also in the interior of the grains. In addition, macroscopic and microscopic cracking of the fuel takes place that provides further internal volumes. Consequently, porosity correction factors will always remain a source of uncertainties.

Hypo- and hyperstoichiometric fuel, i.e. fuel with a nonzero value of x has a lower thermal conductivity than stoichiometric fuel since introducing point defects (vacancies or interstitials) increases phonon scattering. As in the case of the porosity correction, the difficulty arises from how to obtain the necessary details of the local stoichiometry. The redistribution of oxygen in nonstoichiometric fuels is not completly understood. Chemical processes certainly complicate the picture.

Recently, a new dependence of λ was found which results from an obviously structural change of the UO_2 fuel near the surface at high burn-up, in the so-called "rim zone". Thus, the burn-up effect consists of two contributions: a general degradation in the thermal conductivity of the fuel and the development of the "rim zone" which may act as a thermal barrier.

At the pellet surface of LWR fuel the local burn-up is enhanced due to the build-up of plutonium. Above a local threshold burn-up of 68000 *MWd/tU* microstructural changes (loss of optically definable grain structure, i.e. low angle subgrains on a very fine scale, change of porosity) and a lower dislocation density, lower density of intragranular fission gas bubbles and precipitates was observed [12]. Because of the microstructural changes and the high quantities of fission gas present in this zone, there is a potential for athermal fission gas release. The thermal conductivity of the rim zone is unknown. An increased porosity and a lower concentration of fission gas in the matrix (i.e. a higher concentration of fission gas on the grain boundaries) implies a lower thermal conductivity than would be expected from the burn-up effects discussed above. Since the heat flux density is highest at the pellet surface such a rim effect would further increase fuel temperatures. A first attempt to quantify this effect was undertaken by C. Bagger, M.Mogensen and C.T.Walker. [13]. The authors used direct centre line temperature measurements, temperature "markers" (grain growth and xenon diffusion data) to construct a radial temperature profile. From known boundary conditions they concluded that the thermal conductivity of the rim zone is considerable lower (factor 5 to 10) than in the rest of the fuel, thus the rim zone acts as thermal barrier. This finding, however, needs further clarification.

3.1.2 Heat transfer coefficient between fuel and cladding

The heat transfer coefficient between fuel and cladding (gap conductance) is an important contributor defining the temperature of the fuel. At high burn-up where the gap is closed, the influence is not as pronounced as at the beginning of irradiation. Nevertheless, the gap still acts as a thermal barrier. Gap conductance models depend on temperature, emissivity, gas composition, gas and contact pressure and on surface morphology (roughness, waviness) which may change significantly at high burn-up. Consequently, the surface morphology and composition of LWR fuel and cladding must be known which is especially at high burn-up not the case. The gap conductance at high burn-up needs investigation.

In most fuel rod performance codes, the classical gap conductance model of Ross and Stoute [14] is applied (the contact term is omitted for the sake of simplicity):

$$h_{gas} = \lambda_{gas} / \left(s + a_1 \Delta R + l_{ex} \right) \tag{3}$$

where s is the gap width, ΔR is the sum of surface roughnesses, a_1 a fitting parameter and l_{ex} is the sum of gas extrapolation lengths. An extension of this model is the URGAP model [15] which takes the increase of surface area by the roughness into account:

$$\frac{1}{h_{gap}} = \frac{1}{h_{f,g}} + \frac{1}{h_{cl,g}} + \frac{1}{h_g} \tag{4}$$

where:

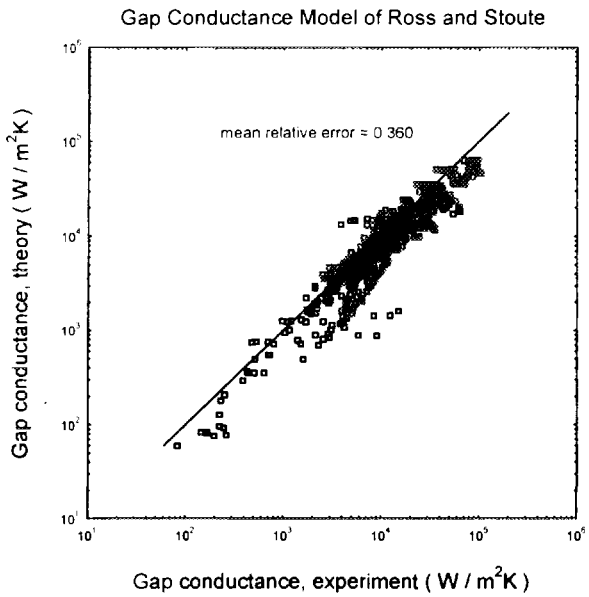

Figure 7 **Comparison of the gap conductance model of Ross and Stoute [14] with experimental data**

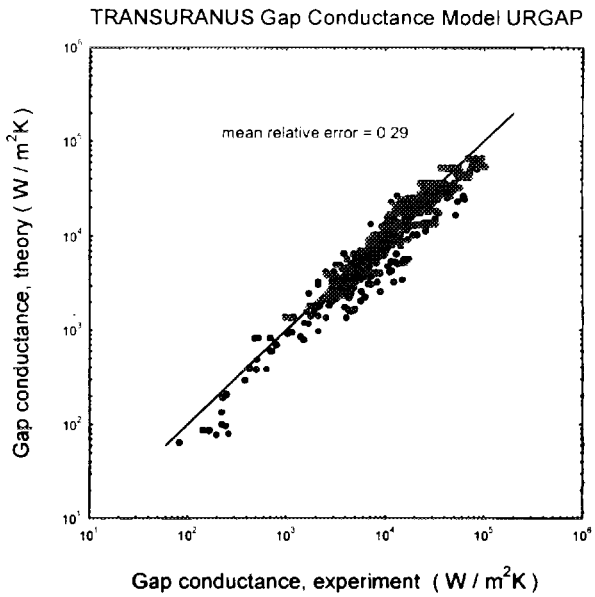

Figure 8 **Comparison of the URGAP gap conductance model [15] with experimental data**

$$h_{i,g} = \frac{\lambda_{gas}\left\{\beta_1\,\beta_2\,\Delta R_i\,(1-\frac{\lambda_{gas}}{\lambda_f})+1\right\}}{\beta_2\,\Delta R_i};\quad i = \text{f,cl}$$

$$h_g = \frac{\lambda_{gas}}{s + l_{ex,f} + l_{ex,cl}}$$

and β_1 and β_2 are fitting parameters.

The gap conductance has been extensively investigated by out-of pile and in-pile experiments. The data base of the Institute for Transuranium Elements consists of approximately 1000 well characterized data covering different material pairings, gas compositions, gas pressures, gap widths, contact pressures and surface roughnesses. Therefore, the error of this important submodel can be investigated since all important input parameters are known. The goal of the following investigation is to find out to what extend theoretical details can be justified by the data. It should be noted that the data bases of other submodels are less extensive and that the uncertainty of gap conductance must be considered as low compared with other submodels.

Both, the standard Ross-Stoute model and the URGAP model were investigated. Different options for the thermal conductivity of a gas mixture, the correlation of Lindsay and Bromley [16] and that of Tondon and Saxena [17] were analysed together with different correlations for the gas extrapolation length. A very simple correlation and a more complicated one were analysed which take a standard correlation for accomodation coefficients into account. The results are shown in Table 1 and Figs. 7 and 8. The conclusion is obvious: a good agreement can be obtained with a relatively simple correlation. Details such as the influence of gas accomodation coefficients cannot be inferred from the data simply because the spread is too large. The general conclusion is that beside details of gap conductance model the average relative error is in the range of 30%.

Similar to the discussion of the influence of porosity and stoichiometry on the thermal conductivity of the fuel the problem lies in applying the right data for gap conductance models. At the beginning of the irradiation where the gap is open, the gap size is determined by highly uncertain relocation of the pellet fragments. At high burn-up the integral effect of all irradiation processes, especially gas release (influence on gas composition) and swelling (influence on contact pressure) contribute to an uncertainty of the gap conductance which is certainly larger than the 30% uncertainty of well characterized gap conductance data.

3.1.3 Discussion of the uncertainties of the thermal analysis

The basic equations and most of the dominating processes are well understood. An exception are the properties of the new structure formed at the edge of the fuel ("rim zone") at high burnup which are unknown. For some correlations or models it is possible to identify individual errors. It is interesting to note that these individual errors are not often mentioned and it is suggested that these errors should be more addressed. They would form the basis for probabilistc analyses. The more important problem arises when these correlations or models are applied. Most of the important details of the model vary with burnup and it turns out that some of this information is simply lacking during the irradiation. Examples are the pore distribution and morphology or simple gap size, gas composition and pressure. One can imagine that it will be possible to further reduce uncertainties of the thermal

Table 1 Mean relative error of gap conductance of the two gap conductance models and the data base

Mean relative error of gap conductance	Ross and Stoute model	Urgap model
1. Thermal conductivity of gas mixture according to Lindsay and Bromley [16]; accomodation coefficients are taken into account	0.360	0.306
2. Thermal conductivity of gas mixture according to Tondon and Saxena [17]; accomodation coefficients are taken into account	0.312	0.290
3. Thermal conductivity of gas mixture according to Lindsay and Bromley; accomodation coefficients are **not** taken into account	0.360	0.311
4. Thermal conductivity of gas mixture according to Tondon and Saxena; accomodation coefficients are **not** taken into account	0.316	0.293

analysis, however, it will never be possible to completly eliminate them.

3.2 Mechanical Equations

The structural analysis of a fuel rod is governed by three basic mechanical principles: equilibrium, compatibility and constitutive equations. The equilibrium and compatibility equations are the standard equations of structural analysis. The constitutive equations, also called stress-strain relations or as material equations, are well known in their simplest form as Hooke's law. A further specialisation of the generalised Hooke's law is the case in which the material is assumed to be linear, isotropic and elastic. The theory of an elastic-plasticity solid is already a very complex and broad subject, however, the fuel behaviour is much more complex due to local swelling, densification and cracking. The fuel must be considered as anisotropic, with different behaviour under tension and compression. Plastic deformations may be caused within short time scales by high stresses and by lower stresses within large time scales. These stresses cause cracking of fuel pellets (macroscopic cracks) but may also cause cracking on a microscopic scale (microcracks). The volume change by densification and swelling is extremely complex since structural changes such as shrinkage of pores, the formation of new bubble population, grain growth and grain decoration and specific irradiation induced damage are involved. How can this complex material behaviour be encapsuled in a constitutive equation?

The presently adopted approach follows the classical approach one by adding strain increments $d\varepsilon_i$ from different mechanisms to obtain the total strain increment $d\varepsilon_{tot}$, for instance:

$$d\varepsilon_{tot} = d\varepsilon_{elastic} + d\varepsilon_{thermal} + d\varepsilon_{plastic} + d\varepsilon_{creep} + \\ + d\varepsilon_{swelling} + d\varepsilon_{densification} + d\varepsilon_{crack-rel} + \cdots \quad (5)$$

where "crack-rel" means a strain increment due to cracking and relocation. Traditionally, plastic and creep strains are distinguished and it is assumed that the volume is kept constant during short time plastic or long time creep deformation.

It is obvious that this concept of material behaviour has some limitations since all contributions are considered as independent. In fact, since all of these proccesses act simultaneously, one of the general difficulties in measuring the behaviour of the fuel during irradiation is to single out specific mechanisms. Clearly, the constitutive equation of fuel needs to be re-evaluated, but it is unknown to the authors whether research is being done in this area.

In the context of this evaluation of uncertainties it is sufficient to briefly discuss the individual contributions. Thermal strains are well known. Swelling may be split into swelling due to solid fission products (volume change $\approx$ 0.7% per atom percent burnup) and swelling due to gaseous fission products. The latter is usually small (volume change $\approx$ 0.1 - 0.3 % per atom percent burnup) but may be significant at temperatures above 1400°C. Thermal and irradiation induced densification is in the range of a few percent depending how stable the fuel is.

Theoretically, the most difficult problem is how to treat the cracked fuel. As can be seen from Eq. (5), crack and relocation may be treated as a fictitious volume change, however, this is only one possible concept. A three-dimensional sketch of a deformed and cracked fuel pellet is shown in Fig. 9. Pellet cracking and relocation can be separated into two mechanisms:

(a) Mechanism 1: The elastic strain prior to cracking is redistributed, i.e. the pellet volume increases and the stress level in the pellet is reduced. This stress reduction depends strongly on the number of cracks and the crack pattern. The following number gives an order of magnitude: 4 to 6 cracks reduce the stress level by a factor of 5 - 10. Fig. 10 shows that not only the stress is reduced but changes also its distribution.

(b) Mechanism 2: depending on the gap size, a relocation, i.e. a gross movement of fuel fragments occurs.

The first mechanism can be modelled whereas the second one by its nature can be treated only empirically. These problems are discussed in greater detail in [18]. It is to be noted that in most situations the second mechanism is by far more important so that details of the first mechanism are masked by

the inevitable uncertainties of the relocation process itself.

A closer analysis of the individual contributions reveals that the total volume change, i.e. the sum of all individual volume changes is uncertain which directly affects gap closure and pellet cladding mechanical interaction. Consequently, due to cracking, relocation and all other effects, the resulting local stresses in the fuel are rather uncertain and great care must therefore be taken if highly stress dependent models are involved.

4 Basic Concepts

In the following chapter three more general concepts are briefly outlined which have been discussed controversially since the beginning of modelling the fuel rod behaviour.

4.1 One-Dimensional Models versus 2-D or 3-D Models

In most of the fuel rod models the theoretical and computational effort is reduced by reducing the geometric dimensions. Relatively simple solutions can be obtained, if the geometric problem is confined to one-dimensional, plane and axisymmetric idealisation (1-D models). A 2-D description (r-θ or r-z coordinates) which is usually based on finite elements techniques significantly increases the computational effort. Even 3-D models are under development [19], however, they are restricted to the analysis of very specific problems. It would be ideal if 3-D analyses would be used to produce adjustment factors for 2-D or even 1-D models [20]. However, the authors are not aware that a systematic attempt has ever been made.

One-Dimentional and 2-D models may have very different characteristic behaviour. From the assumptions made in 1-D models it is clear that deformations of fuel and cladding must differ in both approaches. Fig. 11 shows a schematic comparison of the mechanical interaction between fuel and cladding in a 1-D and a 2-D description. It is evident that local stresses, especially the stresses in the vicinity of the contact area vary significantly. Closer analyses show that local stresses may differ by a factor of 2 to 4. One of the most important limitations of 1-D model is therefore that local mechanical problems cannot be predicted by this approach.

One-dimensional models are well developed and widely used. However, more local details are needed for further optimisation of fuel rods. Therefore a clear trend can be observed: 1-D analyses are augmented by 2-D ones, both approaches being complimentary.

4.2 Steady-State versus Transient Modelling

In the past a "steady-state modelling" was discussed in contrast to a so-called "transient" modelling. Both terms were never clearly defined and different people understood different things by this terminology. This steady-state modelling related to the analysis of normal irradiation behaviour with emphasis on the thermal behaviour. The author suspects that the wording "steady-state modelling" originated from the solution of the simple steady-state heat conduction equation. However, it turned out that the definition of a transient during which specific transient models are to be switched on (and after this transient to be switched off again) is impossible. This means that the development of time-dependent models which also take gradients of loadings or other parameters into account is indispensable in all areas.

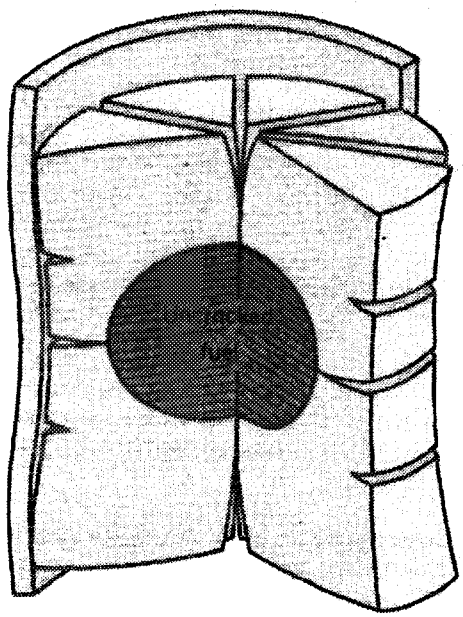

Figure 9 Three-dimensional sketch of a deformed and cracked fuel pellet (from Ref. [18])

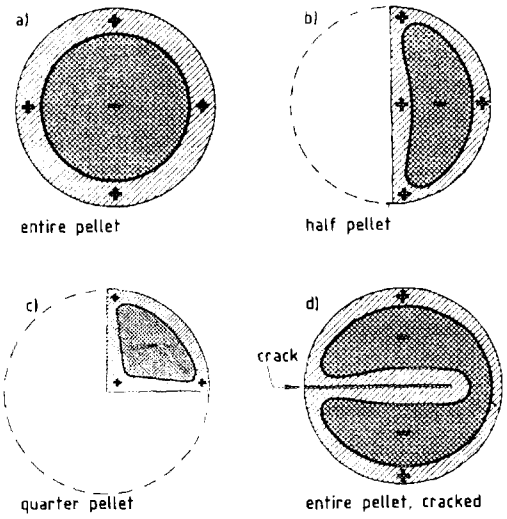

Figure 10 Thermoelastic, hydrostatic stress field in different pellet geometries:
+ tensile stress,
- compressive hydrostatic stress
(results of Mezzi, quoted in Ref. [18])

It is not sufficient to develop a model in an isolated manner, just to describe a particular phenomenon. The model itself should be consistent, reacting in a physically correct manner to the variations in all of the relevant parameters. Such models are certainly more difficult to develop but their usage is straight forward. It should not be forgotten that it was extremely difficult to use some of the simple steady-state models. For instance, years ago, frequently used fission gas release models were of the type:

$$f_i = a_i, \quad \text{if } T_1 \leq T < T_2 \tag{6}$$

where f_i is the fractional fission gas release in the temperature range i between temperatures T_1 and T_2. Eq. (6) can be applied without problems if the fuel temperatures remain constant. For the more realistic case of varying temperatures, Eq. (6) cannot be applied without a specific convention of what amount of gas is to be released in a given time step. Since this convention is nothing else but a pure substitution for a time-dependent, more detailed model, a generally valid convention cannot exist and therefore such simplified models are more or less useless.

4.3 Empirical versus Mechanistic Models

There is no doubt that physical models need to be "correct". But it will be shown below that for nearly all models or processes the most important input parameter such as temperature and local stress exhibit significant uncertainties. Consequently, the complexity of models must be seen in the light of other approximations made. Sometimes it is claimed that detailed models or purely mechanistic models are based upon "first principles". However, it is difficult if not impossible to describe materials behaviour without some free parameters. Fission gas release and swelling is an area in which such attempts were made. Despite highly sophisticated models, the predictions are in almost all cases too uncertain to justify a fuel rod performance code in which all mechanistic models available are included. The relevance of mechanistic models is a more fundamental one since only such detailed models can determine whether the basic processes are understood and what mechanisms are relevant. Fuel rod performance codes used in research may therefore have included complex models whereas standard fuel rod performance codes used preferentially for predictions may include somewhat simplified models which are consistent with the other uncertainties. These type of models are sometimes called "models of adequate complexity".

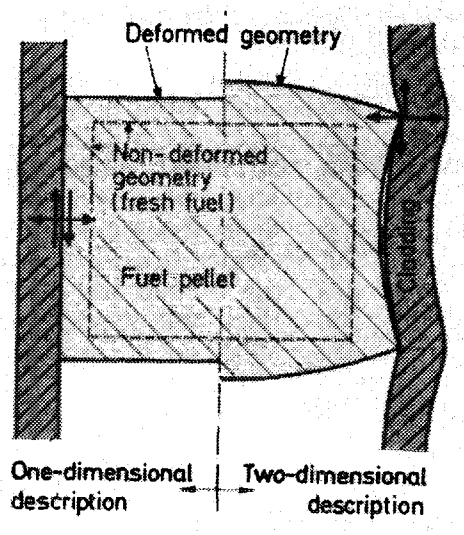

Figure 11 Schematic comparison of the mechanical interactions between fuel and cladding in a one-dimensional (left diagram) and a two-dimensional description (right diagram)

5 Conclusions

Any fuel rod model must include the solution of the heat conduction equation and the principal mechanical equations, i.e. equilibrium and compatibility, together with constitutive equations. These equations form the theoretical structure into which physical models are incorporated. We have identified basic limitations from the different assumptions made for the solution of the governing equations. It is evident that the thermal and the mechanical analysis are strongly coupled and therefore errors are propagated. The individual correlations and processes are also not error free and in only some cases can individual errors be estimated. There is for almost all processes a good understanding of the dominating parameters. However, the unsolved problem is how local quantities such as pores and grain structure, stresses etc. evolve during the irradiation. Thus, the main source of uncertainty lies in wrong input data for local processes.

The problem of determining fission gas release and swelling correctly even after more than 20 years of many specific experiments must be attributed to this category of uncertainties: the more detailed a fission gas release model is, the more local and hence uncertain information is used. For instance, all detailed fission gas release models include a specific gas interlinkage model which determines whether gas can be kept on grain boundaries. However, in order to analyse the interlinkage network, local stresses are needed which exhibit the highest uncertainty. This explains why fission gas release and swelling is so sensitive to alterations in the number of cracks or of the crack structure.

As a final example the centre line predictions of two codes for the FUMEX blind exercise [21] are given in Fig. 12. The selected temperatures cover a wide range of burnup and ratings. Besides the trend to over predict temperatures fair agreement is obtained. This figure is representative of the pres-

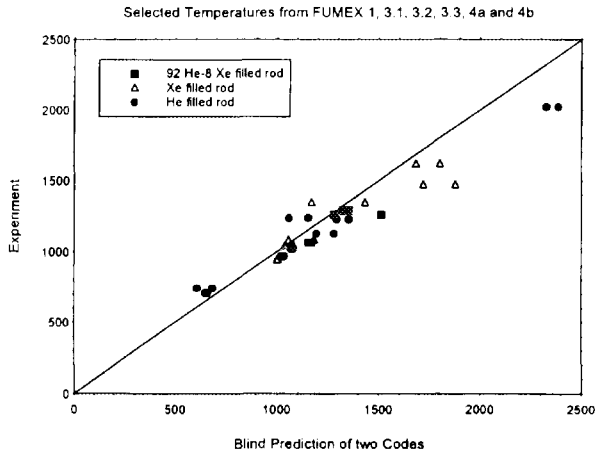

Figure 12 Comparison between measured temperatures and those predicted by two different codes taken from the blind FUMEX code comparison exercise [21]

ent state-of-the-art of the thermal analysis. It should be noted that in order to obtain such an agreement all other models, the mechanical model, physical models (swelling, identification, and fission gas release etc.) and correlations (thermal conductivity, creep etc.) must be correct. It will be very difficult to improve the predictability of fuel performance codes significantly. However, it must also be stated that since the D-COM exercise in 1984 [22], fuel rod performance codes have been improved considerably and must be now considered as mature tools for further optimisation of fuel rods.

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