MODELLING OF AN ACCIDENT TOLERANT FUEL DESIGN USING FEMAXI6

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ABSTRACT

One of trends in the ATF fuel design is to add a secondary phase with high thermal conductivity and low neutron absorption into the UO_2 fuel matrix. In this work, the SiC is selected as an additive since its behaviour under neutron irradiation is well understood. For the assessment of SiC influence on the fuel performance during burnup, the FEMAXI6 code is used. In the work, the source code was modified by introduction the SiC material models of density, thermal conductivity, thermal expansion, heat capacity, Young modulus, and Poisson ratio. The SiC influence on fuel behaviour during normal operation conditions is evaluated using a simple one-pellet model loaded with constant linear heat generation rate and different fractions of SiC are then assumed. The results shows that introduction of SiC decreases fuel centreline temperature, fission gas release, plenum pressure and the pellet expansion due to the swelling is lower as well.

1. Introduction

After the Fukushima accident, new concepts of nuclear fuels [1] are investigated in order to improve the nuclear reactor safety during normal operation and accidental conditions. Such fuels are often called accident tolerant fuels (ATF). During normal operation, they should provide comparable or even better operational characteristics in the form of lower Fission Gas Release (FGR), fuel centerline temperature, and better integrity of the fuel [2]. During the accidental conditions, the main contribution of the ATF is the lower heat accumulated within the fuel pellet due to the lower temperature profile along the pellet radii. It is expected that the lower heat accumulated within the fuel will have a positive impact on early accident management [3].

Before introduction of such a fuel into the commercial market, the vendor has to prove that it is safe to operate this fuel in nuclear reactor. Typically, this is firstly done by numerical simulation at first and then the fuel is tested in a real nuclear reactor (e.g. Kola, ATR, Halden, etc.). Many codes are available for the behaviour prediction of the fuel during burnup, e.g. COPERNIC, TRANSURANUS, and FEMAXI. Since these codes are normally designed for calculation of standard UO_2 fuel, it is necessary to modify these codes in order to cover the influence of the fuel modification [4]. Moreover, it is good to prove fuel operational safety with several different codes by cross checking.

One of the concepts of the ATF is the standard UO_2 nuclear fuel with high content of SiC particles (grains or whiskers). The SiC is favorable from the point of view that it has a high melting point and relatively low neutron absorption [5]. Numerical simulations with modified CAMPUS code [2] have proved that introduction of significant amount of SiC into the UO_2 matrix leads to lower centerline temperature and lower FGR. This paper reconstructs the work done in [2] using the FEMAXI6 code and gives a brief guide how the FEMAXI6 needs to be modified in such cases.

2. The FEMAXI6 code

The FEMAXI6 code is a light water fuel performance code being able to compute many operational fuel characteristics, like e.g.: fuel temperature profile, stresses, strains, and displacements in cladding and pellet (incl. its different components) and also characteristics of fission gas formation and release.

The code consists of two coupled main modules – thermal analysis module and mechanical analysis module. These two modules cover the behaviour of the entire fuel rod. The thermal analysis module solves the tasks related to temperature distribution and fission gas release. The mechanical analysis part deals with the analysis of creep, pellet cladding mechanical interaction, deformation, etc. In each time step, the convergence between temperature and deformation is required as condition for approaching the calculation of the next time step. Analysis of selected single pellet/segment is optional in the FEMAXI6 code [6].

The case being modelled with the FEMAXI6 code is adopted from [2], [7] where an analysis of UO_2-SiC fuel was performed using the CAMPUS code. This model is represented by a fuel pin segment consisting of one fuel pellets surrounded by cladding with defined temperature. The model is depicted in Figure 1. The model operational characteristics are defined as follows. The Linear Heat Generation Rate (LHGR) is zero in the beginning of the simulation, then it is increased to 200 W/m within 3 hours and after that it is kept constant for the period of 1314 days regardless of the SiC volumetric share in UO_2 used. The cladding outer surface temperature is determined as 619 K. In this work, no cladding temperature increment along the axis is assumed. The helium filling pressure is set to 2 MPa.

The model is then used for sensitivity analysis of the SiC influence on the main operational characteristics of fuel pin. In the sensitivity analysis, 0, 5, 10, and 20 vol.% is used as the additive in the standard UO_2 fuel. The SiC is in the form of grains.

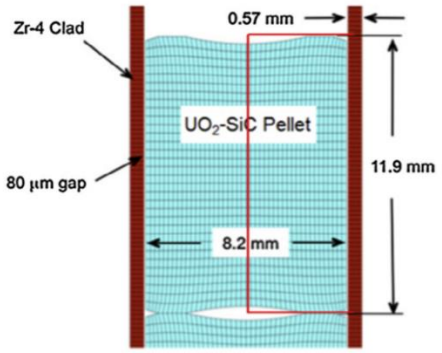

Figure 1: One-pellet model used for assessment of the SiC influence on the operational parameters of UO_2-SiC fuel [2]

It must be emphasized here that the neutronic properties are not of interest of this work. In this work, for example, the increasing SiC volumetric share replaces the amount of UO_2 and thus the reactivity of the fuel decreases. The FEMAXI6 code is, however, not designed to calculate the influence of amount of fissile material on the reactivity. Only some basic routines are introduced in the code for calculation the burnup and heat generation profile depending on the fuel enrichment. So, the decrease in reactivity with increasing SiC content is not reflected in this work. For ones need, the neutronic behaviour of the UO_2-SiC fuel is widely investigated in [8].

3. Methods

The same material models and constants as in [2] are used in this work. However, implementation of all models or its constituents was not possible in all cases since the structure of FEMAXI6 code is different from CAMPUS code. Nevertheless, an effort was exerted here to adjust the calculation conditions as close as possible to that in [2].

In this paper, the UO_2 material models are referred using the FEMAXI6 manual designation in square brackets and they are only listed here since many of them are very well known. Instead of that, the SiC material models are elaborated here in a wider scope. The material models of SiC are mainly adopted from [2] except for density model and thermal expansion model which are taken from [9]. To be in agreement with [2], influence of neutron irradiation on the SiC material properties is neglected.

The UO_2 material models are used as follows: the Lucuta model [10] [IPTHCN=10] for thermal conductivity, MATPRO-11 model [11] [IPTHEX=31,with ATHEX=5.458E-06,RTHEX=7.092E-06] for thermal expansion coefficient, MATPRO-11 model [12] [IPOIS=30] for Poisson's ratio, the NRC model [13] [IDENSF=2] for pellet densification, MATPRO-09 [14] [IFSWEL=2] model for swelling, White & Tucker model [15][IDCNST=2] for fission gas atom diffusion constant equation, MATPRO-11 model [12] [IPLYG=30] for Young's modulus and pellet creep [IPCRP=2].

Density of SiC was assumed as constant and equal to 3210 kg/m^3 [9]. The thermal conductivity function is of the form [16]:

$$\lambda_{SiC} = \begin{cases} 194.776655 - 0.36061185 \cdot \mathrm{T} - 3.3084327 \cdot 10^{-4} \cdot \mathrm{T}^2 - 1.46 \cdot 10^{-7} \cdot \mathrm{T}^{-2} + \\ +2.4758791 \cdot 10^{-11} \cdot \mathrm{T}^4 \ (200\mathrm{K} \le \mathrm{T} \le 1968\mathrm{K}) \\ 24.96986 \ (1968\mathrm{K} \le \mathrm{T} \le 2800\mathrm{K}) \end{cases}$$

where T is in K. The specific heat model is given by:

$$c_{p,SiC} = \begin{cases} 925.62 + 0.3772 \cdot \mathrm{T} - 7.9259 \cdot 10^{-5} \cdot \mathrm{T}^2 - 3.1946 \cdot 10^{7} \cdot \mathrm{T}^{-2} \ (200\mathrm{K} \le \mathrm{T} \le 2400\mathrm{K}) \\ 1365.54238 + 1.379 \cdot 10^{-3} \cdot \mathrm{T} \ (2400\mathrm{K} \le \mathrm{T} \le 2800\mathrm{K}) \end{cases}$$

Thermal expansion coefficient of $4.4 \cdot 10^{-6}$ K^{-1} was used below 1273 K and that of $5.0 \cdot 10^{-6}$ K^{-1} above this temperature [9]. Young's modulus (in MPa) and Poisson ratio are calculated using the following equation:

$$E_{SiC} = 428.3 - 0.04 \cdot \mathrm{e}^{\left(-\frac{962.0}{T}\right)} \cdot \mathrm{T} \ (300\mathrm{K} \le \mathrm{T} \le 2800\mathrm{K})$$

Poisson's ratio model is given by:

$$\nu_{SiC} = 0.160937533 - 2.84171929 \cdot 10^{-6} \cdot \mathrm{T} \ (300\mathrm{K} \le \mathrm{T} \le 2800\mathrm{K})$$

The material properties of UO_2-SiC nuclear fuel were calculated through the rule of mixture where the volumetric share was used as the weight. The thermal conductivity was not calculated using the rule of mixtures but the widely used Hasselman model for composite thermal conductivity [17] was utilized to evaluate the dependency of the UO_2-SiC fuel as a function of SiC volumetric share and temperature. The equation with subscription referring to this paper has the form:

$$\lambda_{UO2-SiC} = \lambda_{UO2} \frac{2\left(\frac{\lambda_{SiC}}{\lambda_{UO2}} - \frac{\lambda_{SiC}}{ah_c} - 1\right)V_p + \frac{\lambda_{SiC}}{\lambda_{UO2}} + 2\frac{\lambda_{SiC}}{ah_c} + 2}{\left(1 - \frac{\lambda_{SiC}}{\lambda_{UO2}} + \frac{\lambda_{SiC}}{ah_c}\right)V_p + \frac{\lambda_{SiC}}{\lambda_{UO2}} + \frac{\lambda_{SiC}}{ah_c} + 2}$$

where a is the grain radii equal to 0.6 μm [18], V_p is the volumetric share of SiC and h_c is the thermal barrier conductance estimated to be approx. $3 \cdot 10^8$ $Wm^{-2}K^{-1}$ using the acoustic mismatch model adopted from [5] and [19].

The above mentioned SiC models were implemented within the following FEMAXI6 functions and subroutines: *PHCAP* (specific heat capacity function), *PTHCON* (pellet thermal conductivity function), *PTHEX* (pellet thermal expansion function), *EXTSTR* (subroutine for calculation of thermal stress on the intra-granular gas bubbles), *FELMOD* (pellet Young's modulus function), *FPOIR* (pellet Poison's ratio function) and density function in *INPUT1* (subroutine which reads the input file). However, it should be mentioned here that reference [2] omits upgrading of some other functions which should be modified as well. For example, the influence of SiC swelling and creep are not included in this reference despite the fact that some models for prediction of the SiC swelling and creep have been published (see ref. [20], [21], [22], [23] e.g.). In this work, the influence of neutron irradiation on the various SiC properties is neglected as well. It is a future aim to publish a paper where the neutron irradiation on the general behaviour of UO_2-SiC nuclear fuel will be asset. This work, where the different properties are treated separately, will be a good starting point for this type of analysis. Preliminary assessment shows that for example degradation of SiC thermal conductivity under neutron irradiation has a large effect on the UO_2-SiC fuel centreline temperature.

When evaluating the results, one should keep in mind that the subroutine *BURNUP* and functions *ADTM*, *ADBU* relate the dependency of burnup and time take the fuel weight as the main input parameter. In this work, these modules were not modified.

In the case of cladding, the models are selected as follows: Zircaloy properties for cladding material [IRM=0], the MATPRO-11 model [24] [CRPEQ=1] for cladding creep, Donaldson model [25] [HTCRP=20] for high temperature creep, modified MATPRO-11 [12] [ICPLAS=2] for cladding plasticity, MATPRO-11 [12] [IZYG=2] model for Young modulus. Ross & Stoute model [26] [IGAPCN=2] is selected for the pellet-gap conductance. If any model of fuel or cladding is not specified here it means that the default FEMAXI6 model is used. For details on the default value, one can see the FEMAXI6 manual [6].

4. Results and discussion

The Figure 2 shows the predicted results of UO_2-SiC fuel behaviour. One can clearly see in Figure 2a that the fuel centerline temperature is effectively reduced with increased SiC share in fuel. The difference in fuel centerline temperature between standard UO_2 fuel and that containing 20 vol. % SiC is 254 °C.

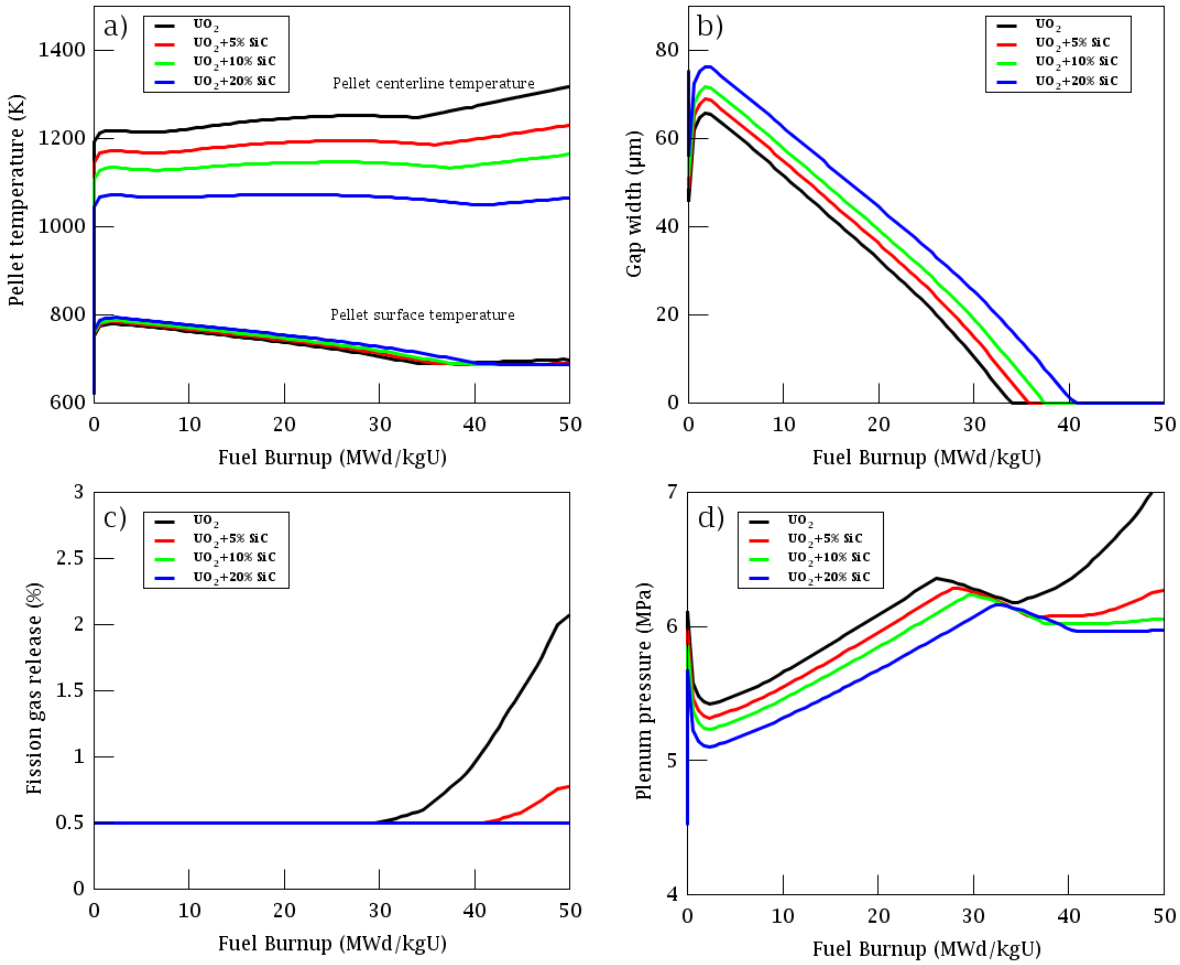

Figure 2: The predicted behaviour of UO_2-SiC fuel during burnup

On the other hand, the pellet surface temperature rises with increasing SiC share before the gap closure (see Figure 2a). This is caused by the reason that SiC has much smaller coefficient of thermal expansion therefore the pellet cladding gap is larger thus working as the thermal barrier resistance. After the gap closure, an opposite phenomena appears. The pellet surface temperature of standard UO_2 fuel rises while the fuels containing SiC have almost the same temperature.

The root of this was found in the gas conductance component of the Ross & Stoute gap conductance model. Even after the gap closure, the gas conductance component plays the major role in the heat transfer. This component is in direct proportion to the thermal conductivity of the gas mixture. The thermal conductivity of the gas mixture is reduced by the presence of Xe and Kr which are introduced to the plenum volume by FGR mechanism. Especially in the case of pure UO_2 fuel, the amount of released Xe and Kr is significant and the gap conductance is reduced and the pellet surface temperature is higher compared to other cases. Next, the solid conductance component is utilized in the Ross & Stoute model but its contribution to the total heat gap conductance is about 15 % at the end of the burnup process.

It should be mentioned here, that the effect of bonding process on the gap conductance is not taken into account using the Ross & Stoute model with option [IGAPCN=2] despite the fact that some models considering the bonding process influence are available in the FEMAXI6 code (options [IGAPCN=5 or 6]). The influence of bonding phenomena on the gap conductance was omitted because the effect of SiC presence on the bonding layer is unclear

and this paper should be considered as the early-stage research and thus physical phenomena modelled are limited to its minimum.

Figure 2c depicts the evolution of FGR. In the FEMAXI6 code, FGR is defined as the ratio of fission gas amount being released from fuel to fission gas amount being generated in the fuel. The amount of generated fission gas depends on LHGR in the FEMAXI6 code and thus is the same for all cases. The diffusion coefficient in the FEMAXI6 code is strongly temperature dependent. It is set to its minimum default value (0.5 %) up to the threshold temperature approx. 1250 K. Above this temperature, the diffusion coefficient starts to rise. The SiC effectively decreases the fuel temperature and thus the FGR is strongly reduced up to the default value even for small share of SiC in the fuel. As the consequence, the generated fission gas atoms remain trapped within the fuel matrix.

Another point worth mentioning is the plenum pressure evolution depicted in Figure 2d. In the early stage, the plenum pressure is governed by thermal expansion and densification of fuel pellets. Later, the fuel swelling reduces the plenum volume and the plenum pressure increases. In the case of standard UO_2 for example, there is a first peak in plenum pressure at approx. 25 MWd/kgU. At this point, the plenum volume reaches its minimum mainly due to the fuel expansion. On the other hand, the plenum volume is then slightly increased by cladding axial growth. After 30 MWd/kgU, the plenum pressure starts to increase again due to increased FGR. The plenum volume becomes constant because cladding axial creep displacement is compensated by the pellet axial swelling and creep components of the axial displacement. A detailed analysis revealed that the final plenum volume is very similar for all cases, but fuels containing higher volumetric shares of SiC pose slightly higher plenum volume due to the smaller pellet axial displacement. This tendency mirrors in the magnitude of plenum pressures of the fuels containing 10 and 20 vol. % SiC which is almost constant after the gap closure due to the very limited FGR.

Regarding the SiC influence on the geometry change during burnup, it can be next stated that the increasing SiC volumetric share decreases the pellet axial growth. The main effect on this has the pellet thermal expansion coefficient which is decreased by the SiC content. Contrary to that, the SiC content reduces the negative UO_2 creep effect. The UO2 creep, according to the MATPRO-11 model, is the function of activation energy, oxygen/metal ratio, fission rate, stress and temperature. As mentioned above, the creep and swelling calculation modules within the FEMAXI6 code were not the subject of modification but they reflect the presence of SiC within the fuel in an indirect way. The SiC volumetric share decreases the centreline fuel temperature and due to different mechanical properties the mechanical stress as well. As the result, the pellet creep is decreased when the SiC is present within the fuel. Regarding the swelling, the MATRO-9 model predicts the swelling ratio based on the fuel centerline temperature only. The first threshold temperature is at 1400 °C and all modelled cases fall below this boundary, therefore the same swelling ratio of 0.28 (%/10^{20}fiss./cm^3) is predicted for all cases.

It should be noted here that the phase stability of the UO_2-SiC system is the most questionable topic. When the UO_2 is sintered with addition of SiC using the SPS sintering method, formation of small voids was observed at the SiC-UO_2 boundary thus forming additional porosity [5]. The question is what will be the development of the voids. It may either remain in its original form or undergo further development. In the worst case scenario, the additional porosity may promote the formation of open porosity and thus increase the FGR. Another potential risk is that the SiC grain will debond from the UO_2 matrix and thus lose contact. In this case, the favourable high thermal conductivity property of the UO_2-SiC

fuel is lost or deteriorated at least and the contribution of the SiC content becomes negative. An extensive material research is next needed in this area.

5. Conclusion

The modification of FEMAXI6 code was performed in this paper in such a way that the UO_2-SiC fuel behaviour during burnup could be performed. The SiC properties (thermal conductivity, density, thermal expansion coefficient, Young's modulus and Poisson's ratio) were implemented into the code. The modified FEMAXI6 code predicts significantly reduced fuel pellet centerline temperature and fission gas release. The reduced fission gas release results in lower plenum pressure. Mainly due to the lower thermal expansion coefficient and lower fuel temperatures of the UO_2-SiC fuel, the presence of SiC content decreases the volume changes during the burnup. However, modifications of FEMAXI6 should be more general, time-burnup dependence modulus are not proper for SiC containing fuel precise modelling. Also SiC creep, SiC swelling and new fission gas release models should be implemented and tested. Authors are proposing to perform calculation benchmark using FEMAXI7, FRAPCON/FRAPTRAN, BISON, and TRANSURANUS nuclear fuel performance codes. There are definitely a large white spots area in UO_2-SiC fuel modelling, so precise benchmark, supported with experimental investigation is really necessary for making a step towards UO_2-SiC fuel fabrication and licensing.

6. Acknowledgment

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