Approaches to simulate destruction of a fuel rod with different fuel types

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Abstract. Due to the revival of interest to the development of fast reactors cooled by liquid metals, the theoretical research for improving their safety is actual. A detailed calculation of all stages of an accident from the beginning to the end requires knowledge of the laws for modelling physical processes occurring in the reactor in case of emergency. The most serious are accidents with core destruction. Simulation of a severe accident in a nuclear reactor is the key element in safety analysis of nuclear power plants. Destruction of fuel rods is one of the most important processes during core degradation that should be calculated. For different types of fuels the mechanisms of the degradation are different too. For example, oxide and metallic fuels usually melt congruently at high temperature, but nitride fuel dissociates. The main objective of the proposed research is to develop models and numerical algorithms for calculation of the destruction of fuel rods with oxide, metallic and nitride fuels. The models of destruction and some calculation results are presented in the paper. The processes are investigated for the first phase of severe accidents, covering the period from the onset of fuel-rod melting to the melt escape from the core center.

1. Introduction

Due to well-established manufacturing and operating technologies, uranium dioxide is the most common nuclear fuel. Along with numerous advantages, dioxide fuel has a number of disadvantages associated with its low thermal conductivity and, as a result, with a large temperature gradient along the radius and a small temperature margin until the melting point. One of the most promising fuels for fast reactors is nitride fuel, which has high density and high thermal conductivity, as well as higher radiation resistance. In contrast to oxide, nitride and metallic fuels do not have such limitations (Figure 1). Moreover, the concept of development of nuclear energy in Russia involves the construction of fast reactors with sodium (BN-1200) and lead (BREST-OD-300) coolants. At the same time, reactor designs involve the use of nitride fuel as the basis.

In comparison with oxide and metal fuels nitride fuels melt congruently only at a temperature equal to 3123 K at a nitrogen pressure over 2.5•10⁵ Pa [1]. The nitrogen pressure in the fuel element is much lower than the mentioned level. So, the destruction of the fuel will occur as a result of the dissociation of nitride according to the reaction:

\[ UN(C) = U + 0.5N_2, \quad U(l) = U(g). \]  

(1)
According to the data presented in the paper [2] the mass loss is determined mainly by evaporation of nitrogen from the surface of uranium nitride at low temperatures, and evaporation of metallic uranium at high temperatures.

Figure 1. Temperature distribution along the radius in fuel pin with different fuel type: 1 – UO$_2$, 2 – UN, 3 – U

2. Basic models for simulating cladding melting and oxide fuel degradation

There are several mechanisms of fuel element destruction in fast reactors with oxide fuel. The first mechanism of fuel disruption is related to abrupt power increase due to TOP (Transient Overpower) accident. Rapid power increase at low heat removal rate may lead to fuel dispersion before the cladding is destroyed. The second mechanism is caused by the cladding melting due to the coolant film drying out during the loss of flow accident or melting of fuel during slow power increase. In the present paper we will describe models for the second mechanism of destruction.

Calculation techniques are described in more detail in [3]. To simulate melting processes, heat equation in the enthalpy formulation is used:

$$\frac{\partial p h}{\partial t} = \nabla (\lambda \nabla T) + Q \ . \ (2)$$

The finite volume method is used for numerical approximation. Due to high power-flux and low operating pressure, sodium vapor velocity may reach more than hundreds of meters per second during the loss of flow accident. This fact may play a significant role in the dynamics of cladding and fuel melt relocation. The simulation of the cladding or fuel melt motion on the surface of the fuel element is carried out by solving the equations of conservation of mass, momentum and energy [4]:

$$\left\{ \begin{array}{l}
\frac{\partial p S}{\partial t} + \frac{\partial p SU}{\partial z} = \Gamma \\
\frac{\partial p SU}{\partial t} + \frac{\partial p S U^2}{\partial z} = -S \frac{\partial p}{\partial z} + \Gamma U_m + p S g s i n \theta + \tau z \Pi \zeta m - \tau w \Pi w \\
\frac{\partial p h S}{\partial t} + \frac{\partial p h S U}{\partial z} = q_w \Pi w + q_z \Pi z + \Gamma h_m
\end{array} \right\} \ (3)$$
The implemented models allow simulating the melt movement on the surface of the fuel rod with good accuracy [5,6]. The example of the calculated distribution of the cladding melts over the surface of the fuel pin with oxide fuel is presented in fig. 2. Coolant velocity is equal to 50 m/s, and heat flux is \(0.5 \times 10^6\) W/m\(^2\) in the presented experiments. Fuel external radius is equal to 0.004 m, and cladding external radius is equal to 0.0045 m.

**Figure 2.** Calculated distribution of the materials: purple – molten cladding, gray – solid cladding, green – solid fuel, blue – coolant vapor. Coolant flows from bottom to top. a) 1.3 s; b) 7.6 s after cladding melting.

As we can see from the figure above, the most part of the melt leaves the active part of the fuel rod during several seconds after the accident starts.

### 3. Basic models for simulating nitride fuel degradation

As it was mentioned above, uranium nitride melts congruently only at high nitrogen pressure under the surface of uranium nitride. Nitride fuels dissociate according to reaction (1). In the temperature range from 2073 K to 2373 K, the rate of mass loss due to dissociation is shown to increase from 0.01% per minute to 0.04% per minute [7]. In the present work, an approximating formula is also obtained for determining the rate of mass loss:

\[
\frac{\partial m}{\partial t} = A + Be^{-Q/RT}
\]  

\(A=1.79\times10^{-3}\) %\/min\(^{-1}\), \(B=-2.904\times10^{10}\) %\/min\(^{-1}\), \(Q=575.5\) kJ/mol.

The amount of the uranium melt can be estimated from the reaction (1) under the assumption that the mass loss is determined by the evaporation of the nitrogen from the surface:

\[
\frac{\partial m_U}{\partial t} = \frac{1}{m_{UN}} \left( \frac{\mu_U}{0.5\mu_{N_2}} \right) \left( A + Be^{-Q/RT} \right).
\]

The amount of the dissociated uranium nitride can be estimated in the same way:

\[
\frac{\partial m_{UN}}{\partial t} = \frac{1}{m_{UN}} \left( \frac{\mu_{UN}}{0.5\mu_{N_2}} \right) \left( A + Be^{-Q/RT} \right).
\]

The characteristic time of the uranium nitride dissociation can be estimated by the relation (6) according to the expression:

\[
\tau = \left( \frac{m_{UN}}{\frac{dm_{UN}}{dt}} \right).
\]
The characteristic time is shown in Figure 3. The dissociation time varies from 1000 min for a temperature of 2400 K, to 2 min for 3000 K.

Fuel temperature is changing during the accident. Therefore, it is interesting to obtain the dependence of the dissociation time on the energy release in the fuel. In this situation, it is necessary to solve the system of equations:

\[
\begin{align*}
\frac{dT}{dt} &= \frac{Q}{\rho C_p} + \frac{\Delta h}{C_p} \frac{\mu_{UN}}{0.5 \mu_{N_2}} (A + Be^{-Q/RT}) \\
\frac{\dot{m}_{UN}}{m_{UN}} &= -\left(\frac{\mu_{UN}}{0.5 \mu_{N_2}}\right) (A + Be^{-Q/RT})
\end{align*}
\]

(8)

The presented system of equations can be solved numerically.

**Figure 3.** Typical dissociation time of uranium nitride depending on temperature

Typical degradation time of uranium nitride in comparison with the melting time of the uranium dioxide and uranium are presented in the Figure 4.

**Figure 4.** Typical degradation time of UN (3), UO$_2$ (2) and U (1) depending on volumetric heat release.
As we can see from Fig.4 nitride fuel is more thermally stable than usual fuel. Uranium melt that forms during degradation can relocate from the active part of the fuel pin. Relocation of the uranium melt is simulated based on the system (3).

4. Basic models for simulating metallic fuel degradation

The melting point of uranium is 1405 K, and the melting temperature of the stainless steel cladding of the fuel rod is equal to 1703 K. Therefore, melting of uranium begins earlier than melting of the shell. Approaches to the simulation of melting and relocation of the uranium melt and stainless steel (SS) cladding are described in section 2.

The uranium melt can destroy the cladding of a fuel rod even before its melting due to eutectic interaction. The eutectic interaction of stainless steel and uranium was studied at the TREAT reactor [8] and in separate experiments [9]. As a result of eutectic interaction, UFe2 compound was formed. The dissolution rate of steel with uranium obtained as a result of studies [8] was characterized by a reversal of the dissolution rate in the region of 1210–1240°C, which is explained by a change in the properties of the UFe2 complex, namely its melting at this temperature (1230°C). To simulate U-SS interaction we use the base reaction of U-Fe interaction:

\[ U + 2Fe = UFe_2. \]  

(9)

According to this reaction we can find the relation between uranium mass change and stainless steel mass change:

\[ \Delta m_U = \frac{\mu_U}{2\mu_U} \Delta m_{SS}. \]  

(10)

Uranium radius change can be found with the help of relation (18) and geometrical scheme shown in Figure 5:

\[ \Delta r_U = R_{SS'} - R_U = \sqrt{R_U^2 - \frac{\mu_U \rho_U}{2\mu_{SS} \rho_U} \left( R_{SS'}^2 - R_U^2 \right) } \]  

(11)

where \( R_{SS'} \) is the new radius of stainless steel that can be calculated with the help of experimental data on the rate of penetration of molten uranium into stainless steel \( U_{SS} [8,9] \).

![Figure 5. Scheme of the U-SS interaction.](image)

The results of the simulation of the stainless steel cladding destruction are presented in Figure 6. The thickness of the cladding is equal to 0.003 m. The temperature of the uranium is different.
Figure 6. Time of destruction of stainless steel cladding for different temperatures.

Conclusion
Approaches to the simulation of fuel rod degradation have been presented in the current paper. Dissociation of the nitride fuel, melting of the dioxide fuel and eutectic interaction between stainless steel and uranium melt have been taken into account during simulation. Some results of the calculation have been also presented.

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References
[1] Olson W, Mulford R 1963 *The Journal of Physical Chemistry* 67(4) 952
[2] Baranov V, Tenishev A, Kuzmin R, et. al 2014 *Annals of Nuclear Energy* 87(2) 784
[3] Usov E, Butov A, Chukhno V 2018 *Atomic Energy* 124(3) 147
[4] Usov E, Butov A, Chukhno V 2018 *Atomic Energy* 124(4) 232
[5] Usov E, Butov A, Chukhno V 2018 *Atomic Energy* 124(5) 287
[6] Butov A, Zhdanov V, Klimonov I, et.al 2019 66(5) 302
[7] Lunev A, Mikhalchik V, Tenishev A, Baranov V 2016 *Journal Nuclear Materials* 475 266
[8] Walter C, Dickerman C. 1964 *Nuclear Science Engineering* 18 518
[9] Walter C, Kelman L 1966 *Journal of Nuclear Materials* 20(3) 314