Heat Transfer Modeling and Computational Experiment for Uranium Dioxide Fuel Fragment Surrounded by Concrete

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Abstract: - The problem is of interest for nuclear power safety and some other fields. Non-stationary two-dimensional boundary task for non-linear heat flow process in cylindrical rod of dioxide uranium surrounded by cylindrical concrete layer is considered with account of the real physical properties of materials depending on temperature, as well as accounting an internal heat generation of radioactive material. The mathematical model of a heat transfer process is realized as computer program for the FLEX PDE platform. Based on the model the computational experiments have been performed and their analysis was made. The results obtained maybe useful by performing the nuclear safety analysis, as well as by model calculations in constructing the passive protection systems against severe accidents at the nuclear power plants.

Keywords: heat transfer process, non-stationary, rod, uranium dioxide, concrete, computational experiment.

1 Problem description and actuality
Non-stationary heat transfer tasks for melt-fuel interaction during severe accidents and other similar problems are of great importance for theory and engineering practices 1-12].

Model physical situations for the fragments of radioactive fuel surrounded by concrete are in focus of the heat transfer processes studied in this paper. Cylindrical configurations of Uranium dioxide in a concrete (UO₂) cover are analyzed in different scenario, various parameters and sizes of the fuel rod and surrounding concrete.

Non-stationary heat transfer processes are considered in a simplified statement about 2-D processes neglecting the changes along the rod. It is assumed that the main changes are in a cross sectional area of the system. And the focus is directed to influence of the real physical properties, which substantially depend on temperature. Such problem is of importance for example in modeling the heat transfer processes during severe accidents at nuclear power plants where high-temperature processes are going fast and a lot of completely different physical situations happen.

2 Basic equations

2.1 The heat flow equations
The heat flow equations for modeling the above-mentioned processes are based on energy conservation law. In dimension form energy conservation equations for Uranium dioxide and concrete are written as follows:

\[ \rho_1 c_1 \frac{dT_1}{dt} = \text{div}(k_1 \cdot \text{grad}T_1) + q_1, \]  
\[ \rho_2 c_2 \frac{dT_2}{dt} = \text{div}(k_2 \cdot \text{grad}T_2), \]  
where \( T \)- temperature (by Kelvin), \( t \)- time, \( \rho \), \( c \), \( k \) – corresponding density, heat capacity and conduction coefficients for Uranium dioxide (1) and concrete (2). \( q \) is intensity of internal heat generation (all values are in SI). For fresh fuel \( q = 10^7 \text{ W/m}^3 \), for spent fuel – about \( q = 2 \times 10^7 \text{ W/m}^3 \).

The equations (1), (2) can be transformed to dimensionless form:

\[ \bar{\rho}_1 \cdot \bar{c}_1 \cdot \frac{\partial \theta}{\partial \bar{t}_{Fo}} = \text{div}(\bar{k}_1 \cdot \text{grad}\theta) + \bar{Q}_1, \]  
\[ \bar{\rho}_2 \cdot \bar{c}_2 \cdot \gamma \cdot \frac{\partial \theta}{\partial \bar{t}_{Fo}} = \text{div}(\bar{k}_2 \cdot \text{grad}\theta), \]  
where the dashed values are dimensionless parameters, with relation to the following their scales, respectively: temperature \( T_0 \), length \( R \), time \( R^2 / a_{\theta} \). \( \theta \) is dimensionless temperature, \( F_0 = ta_{\theta} / R^2 \). Fourier number, \( a = k / (pc) \) - heat diffusivity coefficient, \( R \), \( R \) - the radiuses of concrete and fuel rod, \( Q = q R^2 / (k, T_0) \). \( \gamma = a_{\theta} / a_{\theta} \). Zero indices point the corresponding values by the stated characteristic temperature.
2.2 Boundary and initial conditions

Initial conditions contain the accepted known distribution of all functions at the initial moment of time. Axial symmetry condition for the system is adopted too, which simplifies the boundary 3-D problem making it 2-D. Also equal temperatures and heat fluxes are supposed for the phases at the interfacial boundaries of their contact. For the external surface of the concrete region it is stated heat transfer condition from concrete to a surrounding medium. Thus it yields:

\[ t = 0, \quad T = T_0(x, y), \quad i = 1, 2; \] (5)
\[ x = y = 0, \quad \partial T_1/\partial r = 0; \] (6)
\[ x^2 + y^2 = R_1^2, \quad k_1 \partial T_1/\partial r = k_2 \partial T_2/\partial r; \] (7)
\[ x^2 + y^2 = R_2^2, \quad k_2 \partial T_2/\partial r = -\alpha_2 (T_2 - T_0). \] (8)

Here \( T_e \) is temperature of surrounding medium outside the region occupied by concrete, \( \alpha_2 \) - heat transfer coefficient for concrete, \( r \) - direction by the radiuses of cylinders (normal to cylindrical surfaces of the fuel and concrete).

For dimensionless equations (3), (4) the boundary and initial conditions (5)-(8) are transformed to a form

\[ \bar{t} = 0, \quad \theta = \theta_0(x, y); \] (9)
\[ \bar{x} = \bar{y} = 0, \quad \bar{\partial} \theta/\bar{c}n = 0; \] (10)
\[ \bar{x}^2 + \bar{y}^2 = 1, \quad \beta \bar{\partial} \theta/\bar{c}n = \bar{\partial} \theta_0/\bar{c}n; \] (11)
\[ \bar{x}^2 + \bar{y}^2 = \delta^2, \quad \bar{\partial} \theta_0/\bar{c}n = -\bar{N}u / (\bar{\alpha}_2 \delta) (\theta_0 - \bar{\theta}_0). \] (12)

where \( n \) is normal to surface direction, \( \beta = k_1/k_2 \), \( \bar{\alpha}_2 = k_2 / k_2^0 \), \( \delta = R_2 / R_1 \), \( \bar{N}u = \alpha_2 R_2 / k_2^0 \) - Nusselt number (ratio of external to internal thermal resistance, or heat fluxes due to heat transfer to surrounding compared to conductivity in a concrete layer). Zero indices mean characteristic scales and the parameters by such corresponding scaling values. Thus, the regularities of the physical system are completely determined by \( \bar{F}_0, \bar{N}u \), intensity of internal heat generation \( \bar{Q}_0 \), and simplexes \( \gamma, \delta, \beta \) determining the ratios of heat diffusivities, sizes of the regions (fuel and concrete) and heat conductivity coefficients for fuel and concrete.

3 Physical properties and their dependence on temperature

Diverse combinations of the physical properties substantially depending on temperature predetermine a number of quite different regimes and peculiarities for the high-speed and high-temperature heat flow processes.

For example uncertainties in the corium properties and their dynamic high-speed variation cause big problem by studying the severe accidents’ scenarios. Uncertainties of the hypothetic scenarios are complicated with uncertainties of the corium parameters starting from its content (!).

Physical properties vary in a wide range: density, viscosity, conductivity, surface tension, heat capacity of the liquid and solid phases, heat of phase transition, etc. One can imagine how much different combinations and physical situations are available due to this. Therefore mathematical modeling and computer simulation in a wide range of varying parameters may help to identify the main classes of the systems and their most crucial regimes.

3.1 Physical properties of nuclear fuel, coolant and concrete and their dependence on temperature

According to [13] the heat conductivity, heat capacity and density of nuclear fuel are non-linear functions of temperature, which are polynomial approximated as follows:

\[ k_1 = 10,7 \cdot 9,6 \cdot 10^4 T + 3,43 \cdot 10^6 T^2 - 3,49 \cdot 10^{10} T^3; \] (13)
\[ c_1 = 2209,9 + 2,7773 T - 0,0027 T^2 + 10^6 T^3 - 10^{10} T^4; \] (14)
\[ \rho_1 = 10620-51,473T-2,4621T^2; \] (15)

All approximations are valid in the range of temperatures from about 300 °K to 3000 °K (over melting temperature). More detail data are available from [14-17]. Some of them are given in the Tables 1-3.

3.1.1 Properties of Uranium fuel

Table 1 contains thermodynamic properties of the Uranium dioxide (UO₂) by standard density in solid and liquid states. Table 2 shows comparative physical characteristics of the fuel and some modeling melts used in experimental studies [1-4].

Analysis of the data presented in the Table 1 shows that a lot of different qualitative regimes are available due to changes in properties, which means that by high-speed temperature variation the system behaviors may dramatically change in time.

3.1.2 Properties of mixtures of fuel and other materials

Mixtures of Uranium dioxide UO₂ and different materials: UO₂+BeO, ThO₂, Al, C, Y₂O₃, U₁O₅ etc. versus temperature are presented in the Table 3, where from the properties needed may be chosen.
As it is seen from the Tables 1, 2, one can choose the non-radioactive materials with right properties for modeling the severe accidents scenarios or some other physical systems [1-5] for investigation the important crucial phenomena.

### 3.2 Development of the new modeling melts

In some cases researchers need the materials with specific physical properties, which are not available among the known materials. Then such new materials may be developed specially for the goal stated. The new materials have been developed at the Royal Institute of Technology (KTH) for conducting the experimental study of the hypothetical severe accidents' scenarios [4]:

- CaO–B$_2$O$_3$, mass fraction (wt/o) 30:70, density ~2500, melting temperature: 1250 °K (solids), 1300 °K (liquidus), crucible: carbon steel or stainless steel (better), bad SiC;
- TiO$_2$–MnO$_2$, mass fraction (wt/o) 18.7:81.3, mol fraction (m/o) 20:80, density ~4500, melting temperature: 1620 °C (liquids), 1520 °K (solids); TiO$_2$ (25kg), MnO$_2$ (50kg), crucible: carbon steel or stainless steel (better), bad SiC;
Table 3. Physical properties of the mixtures of Uranium dioxide UO$_2$ with different materials: UO$_2$+BeO, ThO$_2$, Al, C, Y$_2$O$_3$, U$_3$O$_8$, etc.

- WO$_3$-CaO eutectics, mass fraction (wt/o) 92.5:7.5, mol fraction (m/o) 75:25, density ~6250, melting temperature: 1470 °K (liquidus), 1410 °K (solidus), crucible: good with SiC.

4 Computational experiment
Modeling and computer simulation have been made in a wide range of the varying parameters to reveal the regularities and important features of the heat flow processes in the system described above.

Dynamics of the system’s evolution was determined from solution of the boundary task for equations (3), (4) with the boundary and initial conditions (9)-(12) accounting the non-linear physical properties and approximations (13)-(15).

4.1 The initial data for numerical solution of the boundary task
The initial temperature of the system was taken 20°C (293°K), temperature of the fuel rod 2500°C (2773°K).

The second situation was chosen as initial temperature of the system 20°C but in a center of the fuel rod there is placed point source with a temperature 2500°C. The task is solved with account of the physical properties of the Uranium oxide from temperature.

4.2 Computer program for numerical solution of the boundary task
For numerical solution of the boundary task (3), (4), (9)-(15) the following computer program developed and tested has been used:

TITLE 'Transient Conduction in uranium/beton'
SELECT  e=1e-4
VARIABLES  temp
DEFINITIONS
Lx= 1     r=0.1          R1=0.5       Ly= 1
k            rcp           { Conductivity and heat capacity }
0 = 293 temp0= 2773
heat=10^9
INITIAL VALUES  temp= temp0
EQUATIONS
rcp* dt(temp)= div(k*grad(temp))+heat
BOUNDARIES
region 1
k=1.28 rcp=2500*880
start (5,-R1)
region 2
k=-3*10^(-6)*temp^3+3*10^(-6)*temp^2-0.0096*temp+10.679
rcp=10.96*(3*10^(-7)*temp^3-0.0009*temp^2+1.2464*temp+2592.1) start (1,-r) value(temp)= 2773 arc( center= 0.5*Lx,0.5) angle= 360 close [region 3 k= -3*10^(-10)*temp^3+3*10^(-6)*temp^2-0.0096*temp+10.679 rcp=0.01096*(3*10^(-7)*temp^3-0.0009*temp^2+1.2464*temp+2592.1) start (0.5,1) point load(temp)=0 line to (0.5*Lx,0.5*Ly) point value(temp)=temp0} TIME 0 to 36000 PLOTS for t= 60, 300, 1200, 3600, 36000 elevation( temp) from (0.5,Ly/2) to (5,Ly/2) elevation( fluxd_x) from (0.5,Ly/2) to (5,Ly/2) surface(temp) HISTORIES history( temp) at (0.1*Lx,Ly/2) at (0.2*Lx,Ly/2) at (0.3*Lx,Ly/2) at (0.4*Lx,Ly/2) at (0.5*Lx,Ly/2) at (0.6*Lx,Ly/2) at (0.7*Lx,Ly/2) at (0.8*Lx,Ly/2) END

The computatio was performed in the FLEX PDE platform.

4.3 The results of computations

The situations considered were chosen as follows. Radioactive cylindrical fuel rod surrounded by concrete is prone to heat transfer from the external surface of the concrete (air or water). By different sizes the situation may vary a lot, e.g. fuel rod of 1 cm radius or massive fuel rod 10 sm radius and higher, inside the thin concrete shell or thick concrete layer, etc.

Also the other physical situations were considered, for example, cooling of the hot fuel massive with weak internal heat generation (corium with low concentration of the spent fuel or similar) surrounded by thin or thick concrete layer. The computer simulations allowed revealing some very interesting features of the processes, which may be useful for diverse engineering applications including nuclear power safety problems.

4.3.1 Corium inside the thick concrete layer by weak internal heat generation

This model task was considered for the initial temperature of concrete 293 °K and corium 2773 °K. Heat conductivity of the concrete was taken equal to 1.28 W/(m·°K), density and specific heat capacity coefficient, respectively, 2500 kg/m³ and 880 J/(kg·°K). It is supposed that weak effect of internal heat generation supplies constant temperature on the external surface of corium rod, which has initial temperature the same as temperature of the surrounding concrete massive. Such simplification of the problem statement allows comparably easy modeling of the conjugated boundary task. It allows estimating the intensity of a heat spreading from the narrow surface region of the cylindrical fuel rod into surrounding medium. Some results of computations are presented in Figs 1-4.

The numerical computational grid is presented in Fig. 1. It consists of two circles in the cross section of the physical system of interest: internal fuel rod and external concrete layer.

Fig. 1 The numerical computational grid for the conjugated domain of fuel rod and surrounding concrete layer

Fig. 2 Distribution of temperature by cross section of fuel and concrete for $t = 1$ h

The grid contains huge number of elements built by the method of triangulation. It is adaptively rebuilt at each time step according to the local gradients of parameters. Therefore the most condensed it is in the sub domains with the highest gradients of functions, e.g. on the interface between fuel and concrete where the temperature gradients are the highest. In the rest of the numerical domain the grid nodes are not so small.
This computation was made for the fuel radius 1 m and concrete layer radius 5 m. Figs 2-4 show the results for the time from 1 to 100 hours, respectively. Similar picture is observed for the radiuses 0.1 and 0.5 m by time \( t = 0.01 \) h (0.6 minutes) and for thin rod 0.01 m surrounded by concrete layer of 0.05 m thickness the same picture is observed by \( t = 0.0001 \) h. For this time interval the fuel temperature becomes nearly uniform in the whole region while the concrete still remains cold.

Thus, large scale system is reaching the stationary regime in one day. By this process concrete just starts to warm up getting the temperature 500 \(^\circ\)K on a distance about 2 m from the center. For the medium and large scale systems the same status is reached in one hour and 0.01 h, respectively. And only in 1000 hours the temperature front gets 400 \(^\circ\)K by external concrete surface, so that the concrete under such situation firmly serves as heat insulation for fuel rod.

This situation has local character and may be applied for disposal of nuclear waste with low activity.

The large scale system reaches the temperature 2000 \(^\circ\)K on the external surface of concrete for ten thousand hours, which is the critical state. The corresponding times for medium and large scale systems are 100 and 1 h.

4.3.2 The case of the same thickness of corium and concrete layers

If the concrete layer’s thickness equal to the radius of fuel cylinder, the temperature inside the fuel massive becomes uniform approximately in 100 h, and then the temperature of a concrete is going fast linearly up 800 \(^\circ\)K on its external surface.

4.3.3 High temperature in a form of Delta-function in a center of fuel rod

For this case the corresponding computer program is given below, where the domain of the fuel rod is divided into two sub domains, one of which is just point with a high temperature:

```
TITLE 'Transient Conduction in uranium/beton'
SELECT errlim= 1e-4
VARIABLES   temp
DEFINITIONS  
Lx= 1          r=0.1          R1=0.5       Ly= 1
k            rcp { Conductivity and heat capacity } 
tempi= 20      temp0= 2500     fluxd_x= -k*dx(temp)
INITIAL VALUES   temp= tempi
EQUATIONS   div[-k*grad(temp)]+ rcp* dt(temp)= 0
BOUNDARIES   region 1
             k=128   rcp=2000*840
             start (5.-R1)
             arc( center= 0.5*Lx,0.5) angle= 360 close
             region 2
             k=-3*10^(-10)*temp^3+3*10^(-6)*temp^2-
             0.0096*temp+10.679
             rcp=10.96*(3*10^(-7)*temp^3-
             0.0009*temp^2+1.2464*temp+2592.1)
             start (1.-r)
               arc( center= 0.5*Lx,0.5) angle= 360 close
             region 3
             k= -3*10^(-10)*temp^3+3*10^(-6)*temp^2-
             0.0096*temp+10.679
             rcp=0.96*(3*10^(-7)*temp^3-
             0.0009*temp^2+1.2464*temp+2592.1)
             start (0.5,1) point load(temp)=0 line to (0.5*Lx,0.5*Ly)
             point value(temp)=temp0
TIME   0 to 36000
```
The results of computations are presented in Figs 5-7. Fig. 6 shows that for the large scale system temperature distribution in a form of Delta-function still remains in the center of fuel massive even after 10 hours. Fig. 5 evidences that in this case the temperature is smooth by its decrease in all region. Therefore numerical grid is more regular too, without peculiar regions of sharp gradients and grid condensing.

The Fig. 7 shows that even in a layer of fuel massive the temperature is changing comparably slowly, while in the main part of the region occupied by concrete the temperature is practically stable.
4.3.4 Fuel massive with internal heat generation surrounded by concrete

The corresponding computer program in the platform FLEX PDE is given below:

```
TITLE 'Transient Conduction in uranium/beton'
SELECT errlim = 1e-4
VARIABLES temp
DEFINITIONS
  Lx= 1 r=0.1 R1=0.5 Ly= 1 k  rcp {Conductivity and heat capacity}  heat= 0  tempi=293 temp0= 2773 fluxd_x= -k*dx(temp) fluxd_y= -k*dy(temp)
INITIAL VALUES
  temp= 1500
EQUATIONS
  rcp*dt(temp)+ dx( fluxd_x)+dy(fluxd_y)=heat
BOUNDARIES
  region 2
    heat=0 k=1.28 rcp=2500*880
    start (5.0) natural(temp)=(10/1.28)*(temp-tempi)
    arc( center= 0,0) angle= 360 close
  region 1
    heat=10^4 k=-3*10^(-10)*temp^3+3*10^(-6)*temp^2-0.0096*temp+10.679
    rcp=10.96*(3*10^(-7)*temp^3-0.0009*temp^2+1.2464*temp+2592.1)
    start (1.0) arc( center= 0,0) angle= 360 close
  region 3
    k=-3*10^(-10)*temp^3+3*10^(-6)*temp^2-0.0096*temp+10.679  rcp=0.01096*(3*10^(-7)*temp^3-0.0009*temp^2+1.2464*temp+2592.1)
    start (0.0) point natural (temp)=0
TIME
  0 to 3600
PLOTS
  for t= 60, 300, 1200, 3600
  elevation( temp) from (0.5,Ly/2) to (5,Ly/2)
  surface(temp)
HISTORY
  history( temp) at (0.1*Lx,Ly/2) at (0.2*Lx,Ly/2) at (0.3*Lx,Ly/2) at (0.4*Lx,Ly/2) at (0.5*Lx,Ly/2) at (0.6*Lx,Ly/2) at (0.7*Lx,Ly/2) at (0.8*Lx,Ly/2)
END
```

The calculations were performed by \( q=10^4 \) (fuel massive has total radioactivity like a spent fuel, e.g. corium with a lot of mixture) for two cases of the initial temperature in the region (293 and 1500 °K), for the systems of large, medium and small scales. Numerical domain is shown in Fig. 11:

where from follows that maximal condensing the triangle grid nodes corresponds to the boundaries of the domain with the maximal temperature gradients.

Some of the results obtained are presented below. Thus, the results for initial temperature 293 °K are shown in Figs. 12-14:

As seen from the Fig. 12, the temperature in a center of fuel massive is growing from 293 °K to 1200 °K in 10 hours in a large scale system (correspondingly in 0.1 h in a system of medium scale and in 0.001 h – in a small scale system), on the boundary interface with concrete – up to 500 °K, and a concrete is heated from 293 to 500 °K only at a distance less than 10% from boundary with fuel massive.

In hundred hours fuel in the center is heated up and melted, at the boundary has the temperature на границе имеет температуру 1500 °K. Concrete...
keeps the initial low temperature on a distance from 2.5 to 5 m (in a system of medium scale – from 0.25 to 0.5 m). The dynamics of the temperature field in time in different cross sections of the fuel region is shown in Fig. 14:

Fig. 13 Temperature field by cross section of the fuel massive and surrounding concrete at $t = 100\ h$

Fig. 14 Evolution of the temperature field by cross section of a fuel in time from 0 to $t = 10\ h$

Similar results for initial temperature 1500 °K are given in Figs 15-19. From Figs 15, 16 follows that in 10 h the temperature in a center of fuel massive overwhelms the melting point, while on the boundary it is just 1700 °K. Concrete is heated up to 1700 °K in a thin boundary layer, with nearly the initial temperature 1500 °K in the rest of region. Only on the external boundary of the layer concrete is cooled down from 1500 to 800 °K (temperature of surrounding medium) on a distance of 0.5 m (10% of thickness of the layer).

The clear understanding of the processes give spatial temperature distributions for fuel massive and concrete done in Figs 17, 18. Difference in temperature behaviors of the fuel with time from the center to the boundary presents Fig. 19.

5 Conclusions
An analysis of the non-stationary non-linear heat transfer processes for the different scales and physical situation of the fuel rod surrounded by concrete has been done with account of real physical properties dependent on temperature. Influence of all mentioned factors was investigated and regularities of the system revealed. The results obtained are
useful both for the theory and engineering applications, e.g. in analysis of the hypothetic severe accident scenarios at the nuclear power plants and in other important applications.

References: