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**Numerical study of uncertainties in the
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Аннотация

Рассматривается проблема анализа неопределенностей в моделях барботажа и теплопроводности внутрь бетона. Проводится численное исследование с помощью компьютерных кодов на основании результатов натуральных экспериментов ACE MCCI TEST L4, MACE M1, BETA V7.1. В качестве основных результатов представлены временные зависимости таких параметров как: глубина эрозии, толщина корки, средняя температура расплава. Полученные результаты показывают важность рассматриваемых моделей и их влияние на интегральные характеристики процесса MCCI.

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Numerical study of uncertainties in the models of heat transfer at MCCI

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Abstract

The problem of the analysis of the uncertainties in the bubble models and the heat conductivity into concrete is being observed. Numerical investigation is being done with the help of computer codes on the basis of the results of the natural experiments ACE MCCI TEST L4, MACE M1, BETA V7.1. Time dependences of such parameters as the depth of erosion, the thickness of the crust, the average temperature of the melt are presented as the main results. The obtained results show the importance of the models being observed and their influence on the integral characteristics of the MCCI process.

1 Introduction

The course of the severe accidents at the NPP is accompanied by the melting of the heat generating elements and without proper preventing measures it may lead to a full core melt, to the melt through of the reactor's vessel and to the fall of the molten corium to the concrete base of the shaft. As a result the corium heated up to high temperatures due to residual heat release begins to interact with concrete, destroying it and penetrating into the concrete shaft. Due to the danger of radioactivity outlet from the reactor's containment, much attention is paid to the processes of interaction between the molten corium and concrete (MCCI). Parallel with the theoretical analysis of the main processes at MCCI, natural studies are being conducted in various countries. Some well-known experiments with considerable masses of the melts are being done in the USA in laboratories SANDIA [1] and ARGONNE [2] and in Germany in KFK on the BETA [3] plant.

The idea of these experiments is a detailed investigation of thermal and physico-chemical processes under the interaction of a high temperature melt with various types of concrete. The use of such experimental data in comparison with the results of computational experiments which are fulfilled with the help of programs worked out for the description of this interaction, allows to make more or less detailed testing of these computer codes.

One of the main processes, playing the important role when analyzing and modelling the interaction between the molten core and concrete is the heat transfer in the melt, which depends on the inner structure of the repeated melting of its separate parts. Heat transfer on the boundary melt/concrete is no less important when in the course of concrete decomposition a large amount of gases is being released. These gases form a gaseous film between the molten corium and the concrete base of the reactor. The heat transfer through the film is realized with the help of heat conductivity, convection and radiation. Depending on the intensity of gas release, the regime of a film forming may be laminar and turbulent. While modelling heat transfer on the boundary melt/concrete, it is necessary to consider the possible existence of microconvective boundary layer into the corium near by the boundary. This microconvective boundary layer influences considerably the thermal resistance near by the boundary. As the heat release is reduced and the temperature of the melt decrease to the temperature of solidification, the conditions for crust formation arise on the boundary melt/concrete. It must be emphasized that the formation of crust on the boundaries may lead to considerable redistribution of thermal fluxes which influence significantly such parameters as the depth of erosion, the thickness of the crust, average temperature of the melt and etc.

Chemical reactions in the melt between separate mixture components and gas which bubbles through the melt and also the output of aerosoles and fission products and the change of the residual heat release with such output are of great importance for the analysis. Besides physical processes, the models describing thermodynamic and thermophysical characteristics of the melt's components mixture which take part in the interaction in a wide range of temperatures, influence greatly the receipt of correct numerical results.

Variety of processes and the lack of a detailed and accurate information in many cases raise a lot of approaches for the elaboration of integral physical models and computational programs. Let's mention the programs CORCON [4], WECHSL [3] and RASPLAV [5] among the codes, modelling the processes of core/concrete interaction. The problems are solved in different ways in these programs and this leads to the uncertainty of modelling of transitional and also separately taken processes. At the same time, which analyzing integral characteristics, such as the depth of concrete decomposition, a good agreement experimental data with numerical calculations, performed with the help of various codes, is being observed and this testifies to the conservatism of the models used in this codes.

Uncertainties are understood as insufficient knowledge of properties of complex compounds and processes which take place in the course of contact core/concrete. Insufficient study of some separate process and it's influence on the results of the interaction on the whole is also understood as uncertainty.

In this report one of the possible numerical methods of uncertainty analysis in the models of heat transfer, stipulated by the penetration of gas bubbles through the melt, and heat conductivity in concrete is offered. The uncertainty analysis in these models was done with the help of numerical modelling on the basis of such experiments as: ACE MCCI TEST L4 [2], MACE M1 [6] and BETA V7.1 [3]. The depth of erosion, core average temperature, the temperature on the upper boundary of corium, the thickness of the crust and the rate of it's formation, the rate of burning out of zirconium and other parameters were chosen as the main parameters for the observation.

2 Brief description of the main models of WECHSL version

The program WECHSL describing the quasi-steady stage of core/concrete interaction is guided, is the main, to the calculations for the NPP This program provides one-dimensional and two-dimensional interaction of the active zone residues with concrete for light water reactors. Stratifications of the melt on the oxide layer and metal layer is admitted, besides, the existence of a thin gaseous film on the boundary of interaction between the melt and concrete is supposed to be. WECHSL models assume that when the melt is cooled on the boundaries of interaction with concrete or atmosphere, the existence of the solidification processes is possible, i.e. the formation of solid crust where the heat transfer is stipulated only by heat conductivity. The calculation of solidus temperature T_{sol} and liquidus temperature T_{liq} is of great importance in crust modelling. The triple phase diagram $Fe - Cr - Ni$ is chosen for metals. The influence of other metals on the results of T_{sol} and T_{liq} calculation is ignored. Pseudobinary diagram is used for oxides. In this diagram uranium and zirconium oxides form a high-temperature component and ferrum oxide form low-temperature component. The main chemical reactions reflecting the interaction between the molten metals and gases which are formed in the process of concrete decomposition are also realized in this program.

Code WECHSL is guided to the calculations with one type of concrete. That's why it is impossible to model the experiment with multilayer concrete ACE MCCI TEST L4. In this experiment the basement of the plant was made of silicate concrete except the upper layer in which the serpentine concrete was used. The base of serpentine concrete forms the serpentine mineral (the chemical formula $Mg_3Si_2O_7 * 2H_2O$). The program WECHSL-MOD3 was modified because it was impossible to determine the serpentine mineral in the code. That allowed to take into account correctly $Mg_3Si_2O_7 * 2H_2O$ and MgO oxide, which appears in the result of serpentine mineral decomposition. Besides, the modified code allows to determine not one but two types of concrete all at the same time.

3 Brief description of the main models in the code RASPLAV

The program RASPLAV is determined for two-dimensional modelling of the processes of thermal and mass transfer in the domain of complex form. In this program the problem of heat transfer in two-dimensional (r, z) geometry is being solved. This problem allows to perform detailed modelling of

the processes of formation and repeated melting of crusts, which are being formed near by the boundary of the melt with cooling media. The modelling of phases transitions in the code is done by setting the temperature dependence of thermophysical characteristics. The mechanism of corium elements transfer through the melt and the model of emergence of the products of concrete decomposition are determined in the program. As the result the experiment SURC-4 [1] was modelled more or less in detail. The program supposes the stratification of the melt in layers with the possibility of determining various coefficients of heat transfer on the boundaries between the layers. The models of the main chemical reactions between the molten metals and gases released from the decomposed concrete are observed in the code. The number of layers in concrete (or in some other basement) and the mechanism of heat conductivity in concrete and constructional materials are also considered in this code.

4 Analysis of some peculiarities in the bubble models

One of the most important parameter, defining the heat regime inside melt, is the heat transfer coefficient in the molten corium, which is due to the movement of gas bubbles. In this section the different models for the calculation of the heat transfer coefficient, which depends on the velocity of gases, viscosity and local temperature is being observed.

The following models are realized in the code RASPLAV:
BLOTTNER [7]

$$h = \kappa(g/\nu_l k_l)^{0.33}(0.4\alpha^2)^{0.33}$$

or

$$h = \kappa(g/\nu_l k_l)^{0.33}(0.05\alpha)^{0.33} \quad (1)$$

and

GREENE [8]

$$h = 5.05\kappa(\nu_l/k_l)^{0.8}(V_s/\nu_l r_b)^{0.5}$$

or

$$h = 1.95\kappa(RePr)^{0.72}/r_b. \quad (2)$$

While calculating the heat transfer coefficient the influence of viscosity was taken into account. The following dependence of the of viscosity on temperature was used:

$$\nu(T) = \frac{1 + 0.5f}{(1 - f)^4}, \quad (3)$$

where:

$$f = \frac{T_{liq} - T}{T_{liq} - T_{sol}}.$$

For the first model this influence is essential, but for the second one it is not.

While calculating the heat transfer coefficient in the code WECHSL well known WHERLE model [3] is used:

$$h = 0.0535(g\beta/\nu_l)^{0.33} Pr^{0.417} \Delta T \kappa \gamma,$$

here:

$$\gamma = 1 + 608 \frac{V_s}{u_b} \left(\frac{\rho_L - \rho_H}{\rho_H} \right)^{-0.4265}$$

For the models of mechanical mixture of the corium components the way of approximation of mixture thermal conductivity coefficient is important. While modelling the heat transfer processes in the melt by means of RASPLAV code two possible approximations were considered:

$$\text{the mean arithmetical} \quad \kappa_{tot} = \sum \phi_i \kappa_i \quad (4)$$

and

$$\text{the mean harmonical} \quad 1/\kappa_{tot} = \sum \phi_i / \kappa_i. \quad (5)$$

Since the conductivity coefficients for pure metals and oxides are greatly differ, then while modelling of the full mixing of molten corium the average coefficients, calculated by formula (4) or (5), may be differ to a considerable extent.

The script of experiment MACE-M1 was used for the analysis of the uncertainties in the heat transfer models:

Corium mass	430 kg
Type of corium	PWR
Type of concrete	Limestone/common sand
Concrete dimensions	50.2 * 50.2 * 50.0 cm
Concrete density	2.4 g/cm ³
Initial temperature	2600 K
T _{sol} and T _{liq}	1393/1568 K
Power	100 kW
Pressure	0.1 MPa
Water addition	2.5 cm basemat erosion
Water temperature	300 K

Numerical simulation with help of the code RASPLAV was done for two different values of power, which is supplied in the molten corium: 100 kW and 150 kW.

Calculating experiments showed that values of the depth of concrete erosion are differ one thing from another no greater then 10-15% for the different models and approximations (see fig. 1).

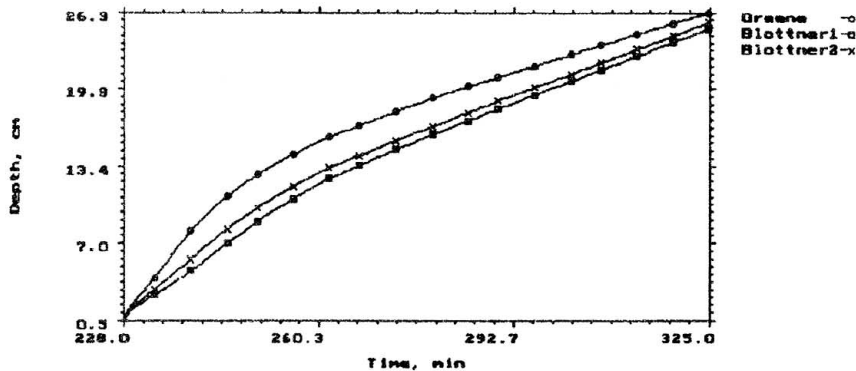


Figure 1. Depth of erosion.

While analyzing the rate of concrete decomposition two regions may be pointed out on the figure 2. The first region corresponds to zirconium burning out and the second region corresponds to quasi-steady process. The rate of concrete decomposition for GREENE model (2) in two times greater then the rate for the other models at the first time interval. At the quasi-steady state phase the erosion rate approximately in 1.4 times less for GREENE model in comparison with others.

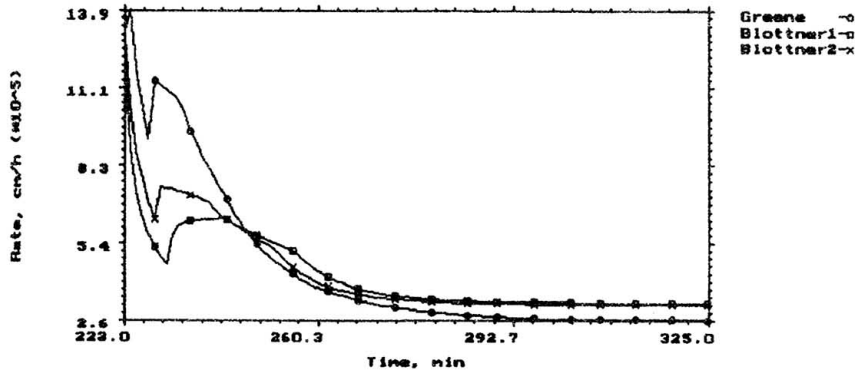


Figure 2: Rate of erosion.

Evolution of the growth crust for the different models are shown in figure 3. The thicknesses of the crust for these models in quasi-steady interval have essential differences. Thus, the thickness of the crust reached 2.04 mm for BLOTTNER model (1) with approximation of the heat conductivity coefficient (4), in the case with other approximation (5) the thickness of crust was 1.28 mm. While using of GREENE model the thickness of the crust was equal 0.216 mm. The time of the crust appearance for these cases are differ one thing from another for 32 minutes.

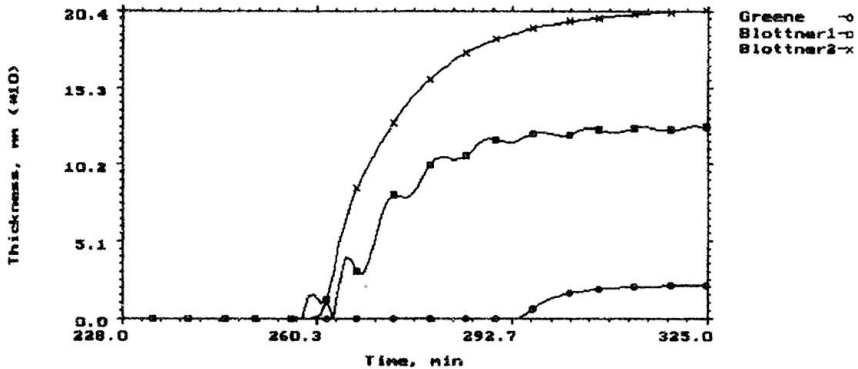


Figure 3: Upper crust thickness.

It's necessary to note that the difference between the average melt temperatures for the different models at the quasi-steady interval is essentially (see fig. 4). The average melt temperature is equal 2045 K for BLOTTNER model with approximation of the heat conductivity coefficient (4), however while using of the approximation (5) it was reached 2139 K. In the case of CREENE model for the temperature the value about 1625 K was received, that close to the solidus temperature 1500 K.

Dependences of the temperature and the heat flux on the upper boundary on time are shown in figures 5 and 6. The analysis of these dependences shows that numerical calculation, using GREENE model, is characterized by the higher temperature and, as a consequence, the more greater heat flux on the upper boundary in quasi-steady time interval.

Thus, summarizing the obtained data, we may state that various approximation of heat conductivity

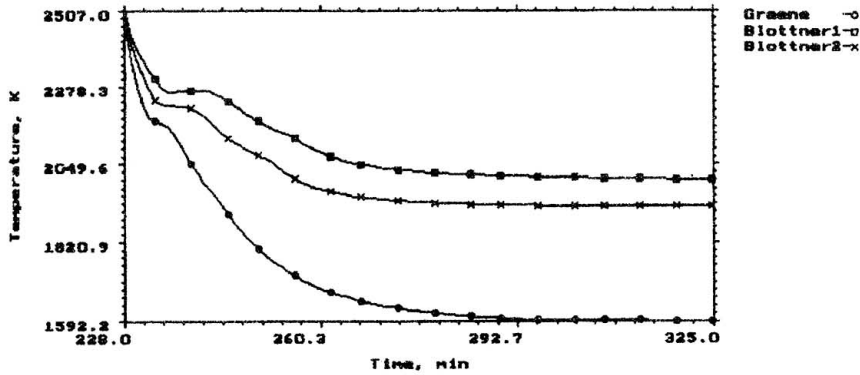


Figure 4: Average melt temperature.

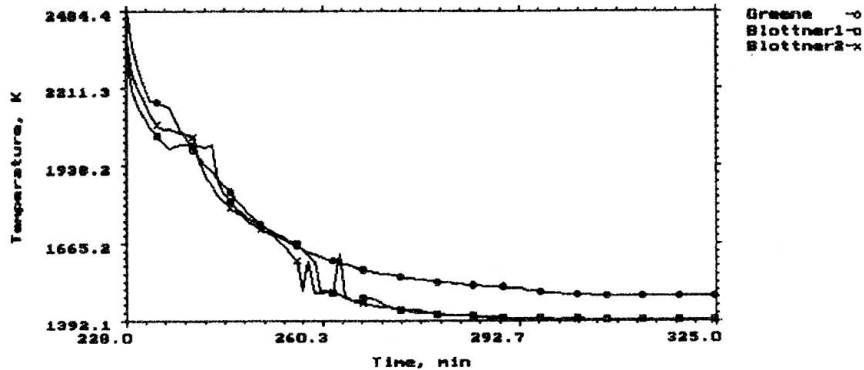


Figure 5: Upper bound temperature.

coefficients doesn't lead to considerable differences of the main parameters. Moreover, the heat transfer coefficient, calculated on the basis of the model GREENE, provides more considerable output of the heat to the upper boundary and a heat flux which is more considerable in the integral sense and as a result, the mean temperature is lower than the temperature obtained by another calculations. This fact may be explained in the following way: the heat transfer doesn't depend on viscosity and local temperature while the heat transfer in the model BLOTTNER reflects such dependence and as a result viscosity plays the main role at such temperatures in the boundary corium layers (the temperature of the boundary layers is close to temperature of solidification).

Calculations with the help of code WECHSL were done with the account of viscosity temperature dependence (3) and without it. In the course of the experiments it was noticed that the depth of concrete decomposition correlates with the viscosity temperature dependence (3). The depth of concrete erosion, ignoring this dependence, was equal to 18.8 cm at the moment of time 8000 sec., and with the account of this dependence, the depth of concrete erosion reached 23 cm during the same time. Besides, the profile of the curve of concrete decomposition, considering the last case, was more gentle (see fig. 7). The designation "Yes" ("No") corresponds to numerical calculations, which was carried out with (without) temperature dependency of viscosity.

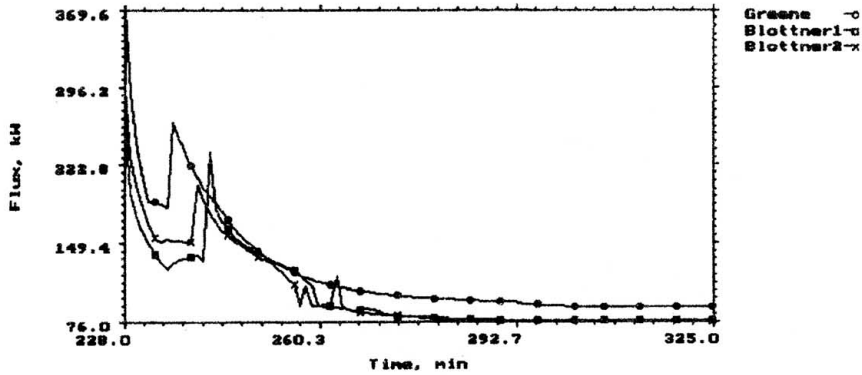


Figure 6: Upper bound flux.

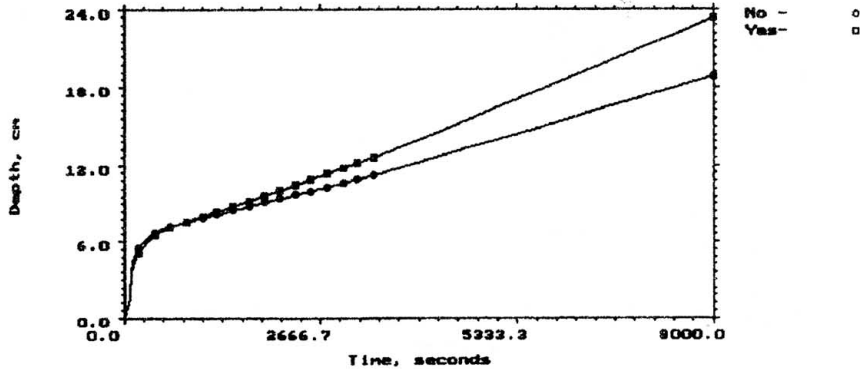


Figure 7: Depth of erosion.

While analyzing the rate of concrete decomposition two regions were pointed out on the diagram (fig. 8). The first region corresponds to zirconium burning out and the second region corresponds to a quasi-steady process. The rate of concrete decomposition in the second region, with the account of viscosity temperature dependence, exceeded the rate of concrete erosion 1.5 times for the calculations ignoring the viscosity temperature dependence.

While studying the growth of the crust (see fig. 9) in the quasi-steady region it was settled that the value of the crust thickness was 4 times greater, when considering the dependence (3), than without it, and the difference in time of the crust formation for these cases was 60 sec.

There was no great difference between the temperatures in the oxide phase for various models in picture 10. In the quasi-steady region, when the dependence (3) was used the temperature in the oxide phase was 1510 K at the moment of time 8000 sec. and in the case when the dependence (3) was ignored the temperature in the oxide phase was 1491 K.

Dependences of the mean temperature and the heat flux on the upper boundary on time are shown in pictures 11 and 12. The analysis of these dependences showed that the numerical calculation, using the model which ignores the viscosity temperature dependence, is characterized by a higher temperature on the upper boundary and as a result of it, the heat flux in the quasi-steady time region is greater than for the

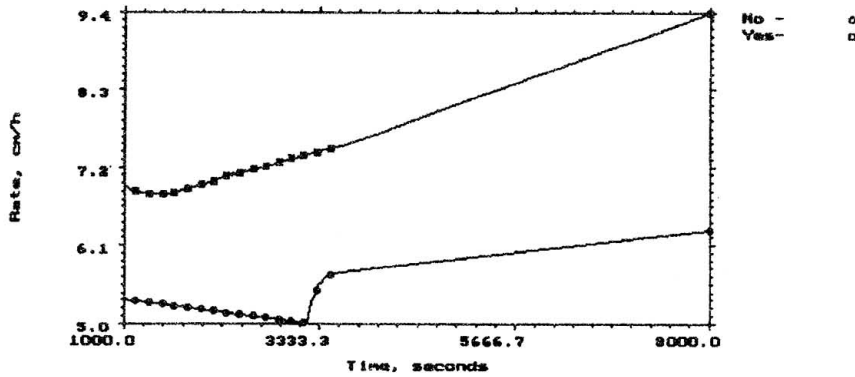


Figure 8: Rate of erosion.

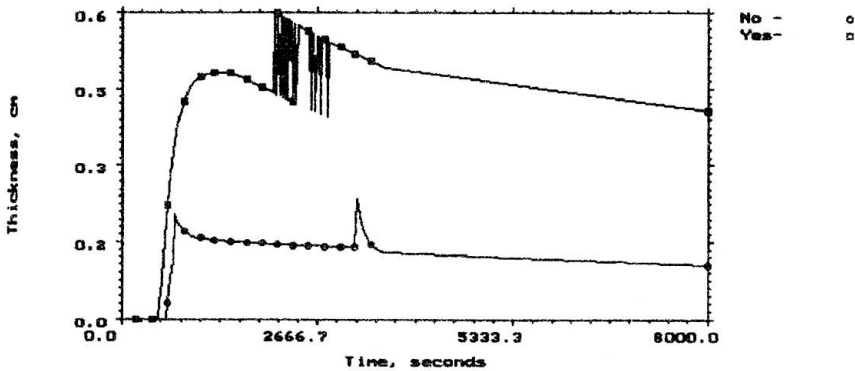


Figure 9: Upper crust thickness.

model which considers it.

5 Analysis of influence of the models of heat conductivity in concrete on integral characteristics

The heat conductivity in concrete plays the essential role in the problems of molten core/concrete interaction. While modelling heat transfer in concrete we observed the following processes. The transition process i.e. the process of preliminary heating of concrete; the process of quasi-steady decomposition of concrete (in case of powerful thermal flow into concrete) and a thermal process, when an insufficient thermal flux for quasi-steady decomposition of concrete is realized on core/concrete boundary. It is supposed in the first and in the last cases that when the coefficient of heat conductivity in concrete is small, the character of heat spreading is of great importance.

The model of direct decomposition of concrete as in codes WECHSL and CORCON and the model which describes this process with the help of the equation of heat conductivity are realized in the computer code RASPLAV.

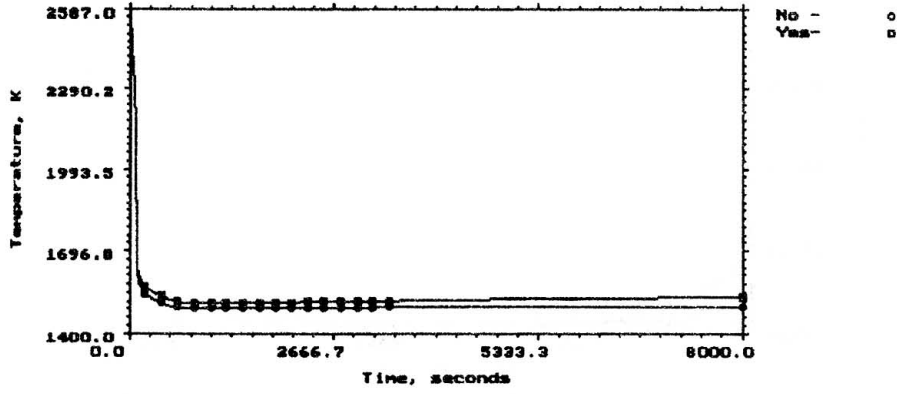


Figure 10: Temperature of oxide phase.

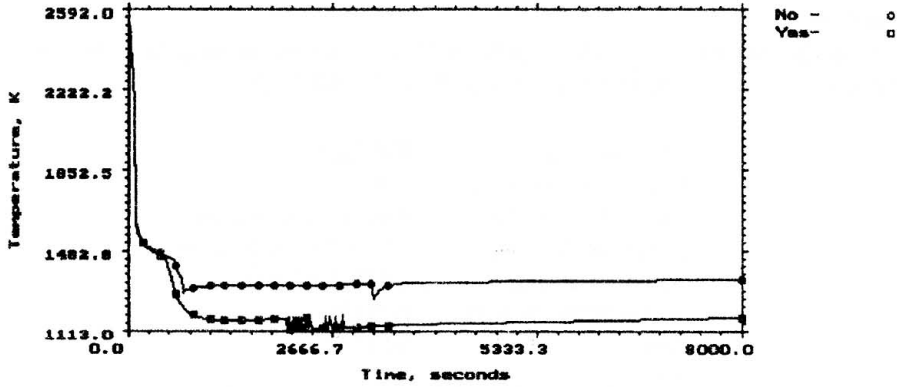


Figure 11: Upper bound temperature.

The heat conductivity in concrete may be described by quasi-one-dimensional equation, supposing that the heat conductivity along the boundary may be ignored:

$$\frac{\partial E}{\partial t} = \frac{\partial}{\partial l} \left(\kappa \frac{\partial T_{conc}}{\partial l} \right),$$

here l is a coordinate along the normal to the boundary of interaction.

Boundary conditions:

$$\kappa \frac{\partial T}{\partial n} = h(T_{bound} - T_{dec})$$

Limitation is imposed on the solution of T_{conc} :

$$T_{conc}(x, y, t) < T_{dec}.$$

Results of the experiment SURC-4 modelling showed that this model allowed to describe the evolution of temperature in concrete and ceramic constructions correctly.

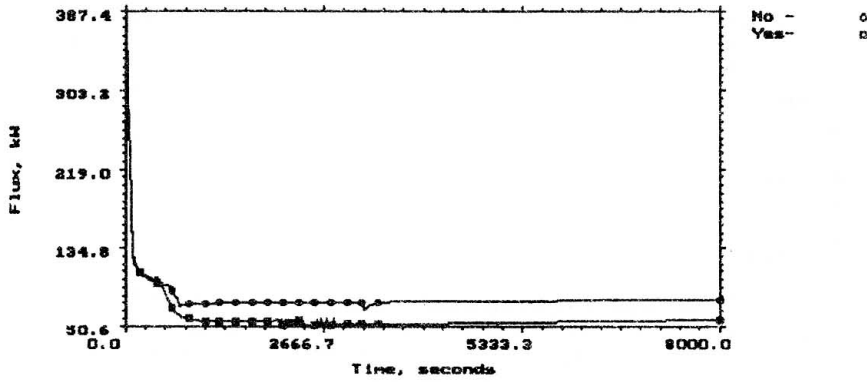


Figure 12: Upper bound flux.

The use of a simple model of direct decomposition of concrete is justified while modelling quasi-steady regime of interaction, on which the code WECHSL is oriented, but this approach may lead to contradictory results.

Inadequacy in the description of the results of MCCI modelling may be shown with the help of the results of numerical calculation of the experiment ACE MCCI TEST L4:

Corium mass	330 kg
Type of corium	PWR
Type of concrete	Serpentine/Silicate
Concrete dimensions	50.2 * 49.3 * 30.5 cm
Concrete density	2.4/2.3 g/cm ³
Initial temperature	2000 K
Power	50 kW

The dependences of the erosion depth, the thickness of the crust and the temperature of the oxide phase on time were used for the observation.

The temperatures of decomposition of the both types of concrete, the surroundings temperature and the solidus temperature were varied.

The analysis of the numerical experiments showed that the depth of erosion of concrete decreased with the increase of the temperature of concrete decomposition.

We got interesting results when we set the following parameters:

T_{dserp}	=	1753	K
T_{dsil}	=	1453	K
E_{dec}	=	2.74	MJ/kg
T_{sol}	=	1200	K
T_{amb}	=	700	K

Vertical erosion, in the case being observed, is approximately constant and it is kept in this state nearly 600 sec. (see fig. 13). However, the temperature on the boundary of the melt (see fig. ??) was no less than the temperature of concrete decomposition that's why using the estimation:

$$h \sim \sqrt{k_{con}\tau} \quad (6)$$

we may estimate the characteristic change of erosion during the mentioned time, which must be no less 3 cm. While comparing the estimations, obtained with the help of the relation (6) with the results of numerical experiment the uncertainty appears.

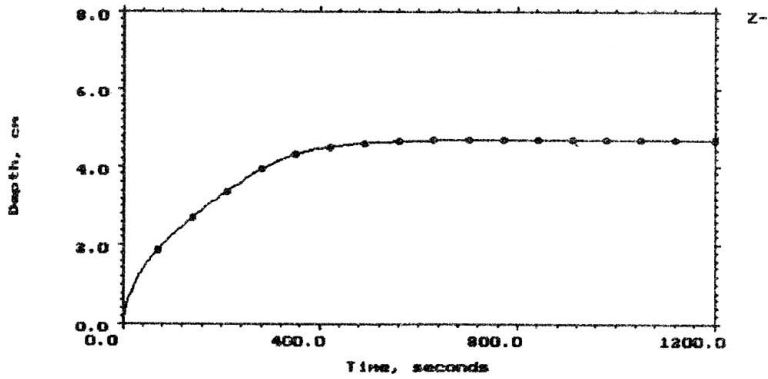


Figure 13: Depth of erosion.

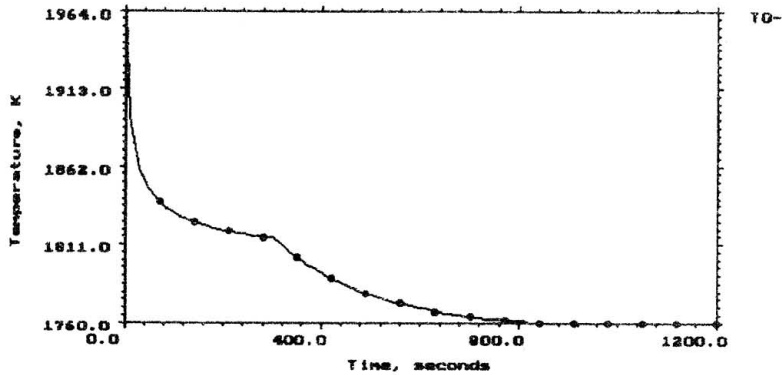


Figure 14: Temperature of oxide phase.

Conclusions

The main conclusions that may be done in the result of numerical analysis of uncertainties are the following:

- viscosity of molten corium and especially its temperature dependence may influence considerably the distribution of the temperature in the melt, the process of crust formation, what in its turn, leads to substantial redistribution of thermal fluxes;
- the model of thermal destruction of concrete must take into account the process of thermal conductivity in concrete that is also necessary for correct determining of gases outcoming in the result of some concrete components decomposition.

Nomenclature

h	—	heat transfer coefficient,
κ	—	heat conductivity coefficient,
k_l	—	thermal diffusivity of the melt,
g	—	free fall acceleration,
ν_l	—	kinematic viscosity,
α	—	void fraction,
V_s	—	superficial gas velocity,
r_b	—	characteristic radius of bubbles,
$Re = (V_s * r_b) / \nu_l$	—	Reynolds number,
$Pr = \nu_l / k_l$	—	Prandtl number,
T_{liq}	—	liquidus temperature,
T_{sol}	—	solidus temperature,
β	—	heat expansion coefficient,
ρ_L	—	low density,
ρ_H	—	high density,
ϕ	—	weight fraction of species i ,
$E = E(T)$	—	enthalpy,
T_{conc}	—	temperature of concrete,
T_{bound}	—	temperature on the boundary,
T_{dec}	—	temperature of concrete decomposition,
T_{dserp}	—	temperature of serpentine concrete decomposition,
T_{dsil}	—	temperature of silicate concrete decomposition,
E_{dec}	—	enthalpy of concrete decomposition,
T_{amb}	—	ambient temperature,
k_{con}	—	thermal diffusivity of the concrete,
τ	—	time.

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