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COMPUTER CODE RASPLAV
FOR MOLTEN CORE - CONCRETE INTERACTION ANALYSES

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ABSTRACT

New computer model for simulation of molten core-concrete interaction is being developed on the basis of numerical solution of two dimension heat transfer problem. The models of boundary conditions, heat transfer in the melt and concrete are described. The main features of code, realized on personal computer like IBM AT or compatibles are considered.

1. Introduction

In risk assessment for the NPP with light water reactors, the accidents with the core melt are of great importance. In spite the probability of such accidents is low, their consequences may be rather severe due to the considerable radioactivity release when the primary circuit is failed. In course of the accident with the core melt the long term interaction of the molten fuel and constructional materials with concrete is quite probable. Such interaction is extremely undesirable, due to the significant increase of pressure under the containment, increase of the atmospheric temperature, possible basemate melting through, the radioactive contamination of the area and ground water .That's why the great attention is played to the analysis of the processes molten/concrete interaction (MCI).

The research work, concerning these problems is performed worldwide and includes a wide range of problems, beginning from the thermal processes analysis in the course of MCI and to the radioactivity release. In some research centers, such as SANDIA [I] in the USA, KfK in FRG [2] and some others, the experiments, concerning the interaction of the melt, simulating the core, with concrete are performed. The goal of these experiments is, on one hand, to receive the experimental information about the materials behavior during the MCI and, on the other hand, all these investigations allow to verify the computers programs, developed for the MCI analysis.

The main processes which are to be modeled, while analyzing the MCI may be divided into three groups:

- thermal-hydraulic processes, including heat balance of the molten core (MC) during the interaction, various processes of heat transfer between separate molten components with the account of

phase transition of the molten components and etc;

- chemical reactions between the molten components and the products of concrete decomposition; these processes are closely connected with processes of gas generation and aerosol release;

- the change of the molten geometry and and the interface between the melt and concrete in the process of decomposition.

The separate problem is the development of models for calculation of thermal-physical properties of the melt components with the account of its composition.

There are several program developed for MCCI analysis, for example, CORCON [3] and WECHSL [4] codes. In both codes quasi-steady state phase of concrete erosion is considered. Due to this circumstance both codes are not always suitable for experiments modeling, especially in case of inductive heating of pool. The second obstacle is that in many experiments, such as experiments carried out in SANDIA laboratory [5], side heat losses are of great importance, so it is very actual for modeling not only core-concrete interaction process, but also general heat transfer problem taking into account the transients in the course of MCCI.

These transients are also important for PWR safety analysis in case of long term MCC interaction.

So, first of all our efforts were directed to model the heat transfer problem not only for molten pool but also for surrounding construction and concrete.

The main differences between the well-known codes CORCON and WECHSL and RASPLAV code are as follows:

- except quasi-steady state interaction code RASPLAV deals with the heat transfer problem in the specific geometry of experimental equipment, and it can simulate not only two dimensional BETA experiments but also one dimension SURC experiments;

heat losses from top pool boundary in codes CORCON and

WECHSL are included by means of key input parameters, so the results depend strongly on user input;

- the transient heat losses, concrete preheating and partial decomposition of concrete also may be simulated by RASPLAV;

- the exact solution of the pool heat transfer problem in RASPLAV code instead of the approximate thin boundary layer model in CORCON and WECHSL codes;

2. Physical models for MCCI

2.1 General Comments

The program RASPLAV is being developed for two-dimensional modeling of heat conductivity processes in the systems with complex geometry and with various heat sources. The main physical processes, simulated in this code are the following:

- 2D heat conductivity taking into consideration phase transitions (melting and vaporization);

  Simulation of phase transitions is done by assuming temperature dependencies of thermal characteristics: heat capacity c and heat conductivity $\varkappa$. Convective heat transfer in the melt with temperature higher than the melting point is simulated by increasing the coefficient of heat conductivity.

- Movement of fuel elements through the melt and also the displacement of concrete decomposition products;

- Realization of various variants of boundary conditions on the outer surfaces and on the inner boundaries for simulating various conditions for the materials cooled by the contact with the boundaries (heat losses due to radiation or boiling of water);

- The program admits stratification of the melt into layers with the possibility of assigning heat transfer coefficients between the layers;

- In the program the models of chemical reactions are also

realized, these include reactions between melted metals and gases, formed during concrete decomposition.

So, in contrast to program CORCON the program RASPLAV allows to calculate transitional processes and also, the developed stage of interaction with concrete with the account of real geometry of the experiment, and various constructional materials, characterized by their own set of thermophisical constants.

In the calculations, given bellow, it was assumed that the melt consisted of two layers - metal layer and oxide layer.

2.2. Pool Structure

The RASPLAV code admits the separation of molten pool into two layers - metal and oxide layers, because numerous experiments have shown the rapid segregation. But also some BETA tests have shown the intermixing of layers in case of high gas release. This current version of RASPLAV code allows two possibilities:

- pool separation into two layers and
- no pool segregation.

This option is chosen now by user and allows to analyze the influence of pool separation on thermal behavior of molten pool.

2.3 Thermal-hydraulics processes

Mathematical aspects of heat transfer problem are to solve two dimensional heat transfer equation in the complex region

$$c\rho \frac{\partial T}{\partial t} = \nabla \text{æ} \nabla T + Q \qquad (1)$$

The equation (1) is solved for

- molten pool (with or without separation);
- surrounding walls (if there are any);
- concrete.

The current version allows to calculate up to six different materials including different layers of molten pool. One medium-atmosphere is modeled specially.

The thermal characteristic of media depend on the following physical properties of media:

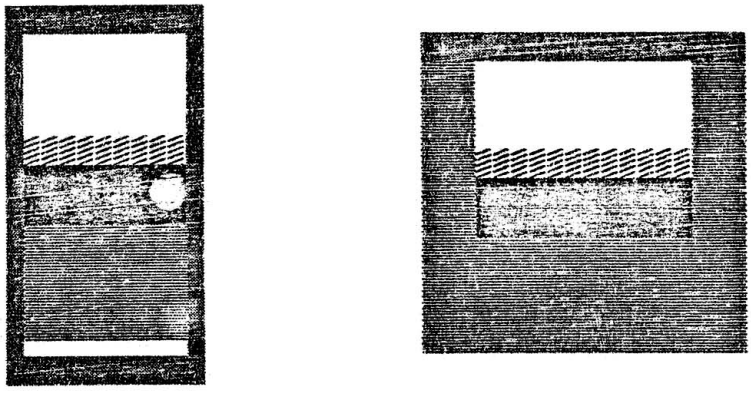
- chemical composition;
- temperature;
- phase conditions.

In order to model phase transitions, we should define first of all melting of different components, the temperature dependence of heat capacity c and heat conductivity $\varkappa$. The latent heat of transition is modeled by increase of heat capacity in the given temperature interval $T_{sol} - T_{liq}$ for each medium. This approach allows melting when the temperature increases higher than T_{sol} and freezing of molten materials in case of temperature decreases below T_{liq}. Appropriate choice of heat conductivity allows modeling of convection by inoreasing of $\varkappa$ when the temperature of the pool is higher than T_{conv}.

The models for calculations of $\varkappa_{conv}$ are being developed now.

2.4 Geometry and boundary conditions

Figure 1 presents the typical geometries allowed in current version. Fig.1a is the typical geometry for modeling SURC experiment, and Fig.1b is for Beta facility.



▒ - oxide layer ▓ - wall material ▓ - concrete

a. b.

Figure 1.

Some geometries for simulation of MCCI

Boundary conditions for different media are as follows:

- on the top boundary of molten pool the radiation is taken into account; in case of closed volumes (like drawn on Fig 1a) the radiation heat exchange between upper pool boundary and surrounding boundaries is possible;

- on the boundary between molten pool and concrete several possibilities are realized now;

  * radiation and convective heat transfer

$$q = \varepsilon\sigma(T_{b1}^4 - T_{b2}^4) + h(T_{b1} - T_{b2})$$

  * heat transfer by conduction; in this case $h \simeq \lambda/\Delta$, where Δ is the distance between contacting cells;

- all other boundaries (molten pool - walls, interlayer boundaries), also allow heat convection or conduction, i.e. the boundary conductions are in the form,

$$q \simeq h(T_{b1} - T_{b2})$$

with possibility of conduction, when $h \simeq \frac{\lambda}{\Delta}$, where heat transfer coefficient is chosen by user input.

It is well-known that heat transfer coefficients in the core-concrete and inter-layer interfaces depend on bubble phenomena in the pool and superficial gas velocity with its proportional to concrete erosion rate. The current version allows to define heat transfer coefficients as a function of different parameters. The gas film model like WECHSL model is included as one of the possibilities. But in general this question is being investigated now to introduce into RASPLAV some models on the bases of experiment modeling.

2.4.1 Gas film model.

To define boundary conditions on the melt-concrete interface the CORCON film model is used []. According to this model flux to concrete is defined by formula (2) and heat transfer coefficient is calculated as follows

$$h = Nu \cdot \frac{æ_G}{\delta},$$

where Nu - Nusselt number, calculated for different flow regimes, δ - gas film thickness, $æ_G$ - gas heat conductivity.

Heat transfer coefficient depends on superficial gas velosity V_s and flow regime in gas film. The following regimes are considered:

Film on the plate surface (inclination of interfasde boundary less than 15°). In this case

$$Nu = Nu_B = 0.804$$

$$\delta_B = 15.05 \cdot Re_B \cdot L^3$$

$$L^3 = \frac{\mu_G^2}{g\rho_G(\rho_L - \rho_G)}$$

$$Re_B = \frac{\rho_G V_s a}{\mu_G} \qquad a = \sqrt{\frac{\sigma_G}{g}(\rho_L - \rho_G)}$$

If the inclination angle greate than 15° the Reynolds number is used for calculations of heat transfer coefficients which is defined as

$$Re_f = \frac{1}{\mu_G r}\int r(1-f)\rho_G V_s dl,$$

where integration along the interface boundary is made. The laminar and turbulent film thickness and corresponding Neussel numbers are calculated:

$$\delta_L = 5.61 \cdot Re_f L^3/\sin\vartheta \qquad \delta_T = 0.046 \cdot Re_f^{7/4} L^3/\sin\vartheta$$

$$Nu_L = 1 \qquad Nu_T = 0.035 \cdot Pr^{1/3} Re_f^{3/4}$$

The final heat transfer coefficients are calculated taking into account the possible mixed regimes of gas film flow. For large inclinations (more than 15°) used formulaes look as follows

$$\delta^3 = \delta_B^3 \cdot \frac{\sin\vartheta_1}{\sin\vartheta} + \max\left(\delta_L^3, \delta_T^3\right)$$

$$Nu = f \cdot Nu_B + (1-f) \cdot \max(Nu_L, Nu_T)$$

f - number characterizing the flux distribution between film and bubbles is changed between 0 and 1 for inclinations $\vartheta_1 < \vartheta < \vartheta_2$.

$$f = \frac{\sin\vartheta_2 - \sin\vartheta}{\sin\vartheta_2 - \sin\vartheta_1}$$

2.5 Chemical reaction in the pool

A lot of chemical reactions can take place between different components in condensed phase in the molten pool.. Now only a part of them is included into codes. These are first of all the reactions between molten metals and gases bubbling though a metal layer.

The current version of RASPLAV code consider the following exothermic reactions between metals and gases released in course of concrete decomposition:

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2O + 7700 \text{ J/g Zr}$$

$$Zr + 2CO_2 \rightarrow ZrO_2 + 2CO + 5900 \text{ J/g Zr}$$

$$2Cr + 3H_2O \rightarrow Cr_2O_3 + 3H_2 + 3500 \text{ J/g Cr}$$

$$2Cr + 3CO_2 \rightarrow Cr_2O_3 + 3CO + 2800 \text{ J/g Cr}$$

These reactions give the main thermal release and should be taken into consideration. Except these reactions which are recognized during the modeling of SURC-4 experiment it was found that the reaction between molten SiO_2 and Zr may be of greate impórtantance.

$$Zr + SiO_2 \rightarrow ZrO_2 + Si + 2100 \text{ J/g Zr}$$

The heat release is about four times smaller than for vapor reaction but the total content of SiO_2 in concrete exceeds the content of H_2O in more than ten times. So, the heat effect of the reaction can be comparable with the heat effect of steam-zirconium reaction.

And the additional heat source due to reactions is calculated by means of formula

$$Q^{Ch}_{H_2O} \simeq \Delta H^{Met}_{H_2O} \dot{V}_{H_2O} \rho_{H_2O}$$

$$Q^{Ch}_{CO_2} \simeq \Delta H^{Met}_{CO_2} \dot{V}_{CO_2} \rho_{CO_2}$$

$$Q^{Ch}_{SiO_2} \simeq \Delta H^{Met}_{SiO_2} \dot{m}_{SiO_2}$$

The index MET is defined by the metal constituent which react with gases at current time and denotes one of the Zr, Cr, Fe.

The total chemical heat is equal to:

$$Q^{Ch} = Q^{Ch}_{CO_2} + Q^{Ch}_{H_2O} + Q^{Ch}_{SiO_2}$$

We do not consider now the reaction between condensed SiO (oxide layer) and Zr (metal layer) because of the chemical kinetics importance for this process which is unknown now.

2.6 Material Properties

The complex melt composition required for adequate modeling is the exact knowledgeof material properties of complex mixtures.

This question is being investigated now and all the material properties can be defined by user input, by means of handbooks for example. We use also temporary models for calculations like models realized in CORCON and WECHSL codes. These auxiliary models refer to simple data base which contains the approximation coefficients for calculations of heat capacity of different materials

$$c = A + B\,T + C\,T^2 + D/T^2$$

where A, B, C, D are the interpolation coefficients depending on temperature interval and phase conditions of the component. The

model realized now is the model of mechanical mixture of components, i.e. the specific heat is calculated by means of formula

$$c = \Sigma\, m_k c^{(k)} / \Sigma\, m_k$$

The heat conductivity $\varkappa$ is defined now by user input.

3.Models of Concrete Erosion

3.1 Concrete decomposition model

Concrete decomposition is a very complicated and complex process.

The models of concrete erosion should consider a lot of physical and chemical processes going on during concrete heating. There are several steps in concrete decomposition when the concrete temperature is increased. The specific concrete processes considered in RASPLAV are presented in Table 1.

Table 1.

Temperature	Processes	Heat ΔQ kJ/mol
400-500 K	H_2O evaporation	39.4
700-800 K	$Ca(OH)_2$ -> $CaO + H_2O$	99.5
1100-1200 K	$CaCO_3$ -> $CaO + CO_2$	165.5
1500-1700 K	Melting	Calculated Value

The temperature intervals depend on concrete type. The heat of different stages of decomposition is included in calculation of heat capacity of concrete. The addition in heat capacity due to these processes is as follows

$$\Delta C_{H_2O}^{evap} = \Delta Q_{H_2O} \alpha_{H_2O} / A_{H_2O}$$

$$\Delta C_{H_2O}^{dehyd} = \Delta Q_{Ca(OH)_2} \alpha_{Ca(OH)_2} / A_{Ca(OH)_2}$$

$$\Delta C_{co_2} = \Delta Q_{co_2} \alpha_{co_2} / A_{co_2}$$

As an input data the user define the decomposition temperature T_{dc} and also solidus and liquidus temperatures.

It is proposed that the final melting of concrete occurred at the temperature T_{dc}. So in calculations the mass of decomposed concrete is

$$\dot{m}_{con} = (1-\alpha_{H_2O}-\alpha_{CO_2}) \dot{V}_{T_{dc}} \rho_{con}$$

where the $\dot{V}_{T_{dc}}$ - is the volume rate of decomposition i.e the volume inside the melting point isotherm.

User input parameter allow to vary mass addition to oxide or metal layers, to take into account layer structure of the pool.

3.2 Gas release model

The gas release from concrete plays an important role for defining heat transfer coefficients on molten pool-concrete interface and also to calculate reaction in the pool . Table 1 shows that decomposition by stages is connected with gas releases. For calculations three parameters are defined: the temperature of bound and free water evaporation, the temperature of $Ca(OH)_2$ decomposition and the temperature of CO_2 release. The proposal is that the gas release is proportional to the volume changes inside the isotherm of dehydration and decarbonization.

$$\dot{m}_{H_2O} = \alpha_{H_2O} \dot{V}_{H_2O} \rho_{con}$$

$$\dot{m}_{CO_2} = \alpha_{CO_2} \dot{V}_{CO_2} \rho_{con}$$

where V_{H_2O} and V_{CO_2} are the volumes inside which the temperature of concrete is greater than T_{H_2O} and T_{CO_2} correspondingly.

This approach means the following physical propositions:

- partially decomposed concrete is permissible for gases;

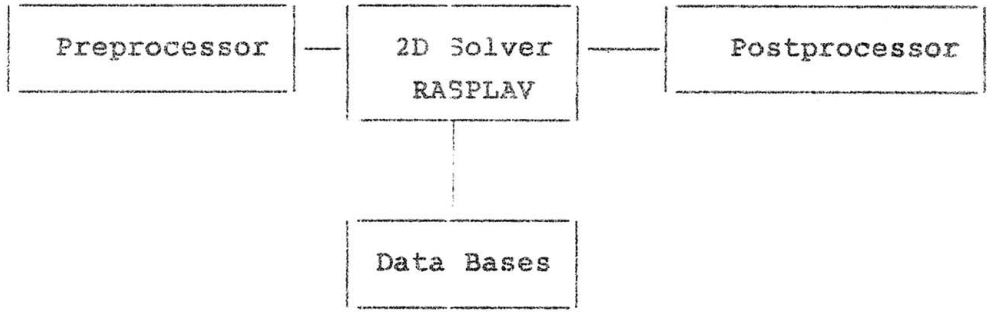
- the gas release is governed by specific temperatures of different stages of concrete decomposition, and do not follow the erosion front; this is especially important for some experiments and long term concrete erosion.

Code structure

The code complex RASPLAV consists of four main parts:

- interactive preprocessor (AUTOGRID)
- 2D heat transfer Solver (RASPLAV)
- Mathematical tools to support data bases
- Postprocessor

The general structure is presumed on fig.



Preprocessor is an interactive code package for automatic grid generation for calculation region. The nonregular meshes are used in calculations. For this purpose the process of grid generation form the correspondence between the real boundaries in physical space and the boundaries in index space. If the calculation region consist of different media then it is necessary to find all the boundaries and establish corresponding boundaries for indexes. After all boundaries are established the mesh is generated. This mesh will not be an orthogonal one. The output preprocessor file (file extension .STK) contains both all the necessary topology aspects of a region and index coordinates of external and internal boundaries.

2D Heat Transfer Solver RASPLAV is a code package for interactive input of different calculation parameters and also the codes for numerical solution of heat conduction equation.

The adaptive nonregular mesh in different media can be built directly in this part of code package but it can also use the grid from AUTOGRID preprocessor.

The possible types of boundary conditions include the boundary condition of the first type and the second type, when the boundary temperature or the boundary heat flux are defined.

The interactive interface allows to define the boundary temperature as a function of time or as a constant, the boundary flux can be defined as a constant, as a table function on temperature and/or time or as an analytical function.

Some boundary conditions are strongly defined:

- on the boundaries between media and atmosphere the radiation heat exchange is necessary;

- on other boundaries the second type of boundary conditions in the form of

$$g = c\ h\ (T_{b1} - T_{b2})$$

are defined.

For the thermal coefficients of heat capacity and heat conductivity it is possible to use the values stored in data bases or these parameters can be defined by user input using interactive windows for data input. All these parameters can be defined as a constant, as a table function or as a analytical function depending on temperature.

The heat source (except additional chemical heat) can also be defined as user input parameter as a function of time or temperature.

2D solver is build using the usual procedure to divide the calculation according to physical processes. The main parts are as follows:

- solving the heat transfer equation for different media, taking into account boundaries conditions;

- generation of new grid (adopt the grid according to melting of concrete, for example);

-interpolation of temperature field from old grid to new one.

This means that during the calculation initially orthogonal grid will be nonorthogonal, so the calculation algorithm realized in RASPLAV is based on economical method of thermal displacement, which will be described later. This method is the generalization of well-known Peacman-Rachford scheme for numerical solution of heat conductivity equation.

The calculation part of code package (solver RASPLAV) realized on C language may be used on any type of computers with C compiler.

When used on PC this code contains small tools for graphic presentation of results: temperature fields, 1D graph for temperature field cross section along x and y axis. The user can interrupt calculation in any moment and see the preliminary results of modeling. The save and restore procedures to continue calculations are also realized.

A lot of information which is useful for core-concrete interaction analysis is included into output files generated during calculations.

Postprocessor for data presentation and data processing allows the following functions:

- quick look of output files and variables stored in it;

- the transformation of data, obtaining an average and integral values (for example, an integral boundaries flux, average temperatures etc.);

- the presentation of results in the form of tables, with their further visualization ;

- graphic presentation.

  * one dimensional graph;

* two dimensional temperature fields presentation;
* 3D presentation of calculations;

- formation and visualization of temporal curves;

- showing graphs of objects in statics and dynamics;

- obtaining of hard copies.

. Postprocessor is realized on PC type of computers, using windows and menu interface which is supported by help files.

Data bases and mathematical tools for data processing are also included into RASPLAV codes. The work of formation and storage data in data bases is not finished now. The main data bases which are planned to be realized are as follows:

- heat capacity tables of different components, taking into according the phase transition points and latent heat;
- heat conductivity;
- thermal characteristics of components;
- chemical data.

General Summary

As it was said earlier the main purposes to make a code package for heat transfer problem. Different parts of this code package allows to input the data, to do calculation and to present results of simulation.

Two parts of code package are oriented for usage on IBM type PC. The central part - 2D heat solver can be used on any type of computers. So, the general procedure of calculation looks as follows:

- PC data input dialog by means of processor;
- main calculations by 2D solver;
- PC interface output of results.

This technology allows to increase the efficiency of data input and data analyses.

Some characteristics of RASPLAV Solver on PC :

- MS DOS operation system (640 KB);
- possible grid about 8 000 cells;
- memory requirement depends on grid used for calculation;
- usual required time about 30 minutes (for grid about 50x100) on PC with 386/387 processor.

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