Numerical simulation of heat and mass transfer processes in a stratified molten pool

Aksenova A.E., Chudanov V.V., Korotkov A.A., Pervichko V.A.,
Semenov V.N., Srtizhov V.F.
IBRAE RAS, Moscow, Russia

Abstract

In the frames of MASCA Project, the theoretical and experimental aspects of heat and mass transfer processes in the stratified system "corium-metal" were studied. The experiments were carried out in the “Rasplav-A-salt” facility. For numerical simulation of the heat exchange in the stratified system “corium-metal” CONV code based on modern algorithms thermal and hydrodynamics and allowing to take into account crust formation on cooled surfaces was used.

The purpose of numerical simulation is an investigation of heat exchange in a stratified salts configuration under experimental requirements, estimation of focusing effect and fluxes on the curvilinear boundary in the lower layer and on the boundary between layers. The results demonstrate, that the CONV code qualitatively and quantitatively predicts heat transfer in the stratified system. This paper presents the basic results of post-test simulation for salt experiments.

1. Introduction

In the frames of MASCA Project one test series was conducted at the RASPLAV salt facility. This test series was conducted in the two liquid layers configuration. The RASPLAV salt facility was designed in a manner to the RASPLAV corium facility (AW-200 tests). The facility represents slice geometry with the characteristic radius of semicircular section of 200 mm. The test wall 20 mm thick was cooled by the secondary salt mixture. The test wall was instrumented with thermocouples, which allowed to measure temperature and heat flux through the test wall. Moreover, the moving frame with many thermocouples provided melt pool throughout the melt volume and boundary layers.

For modeling of heat transfer in the stratified pool, above lower heated salt volume the upper salt layer was settled down. This upper layer of height 40 mm has smaller temperature of melting and is dissociated from lower volume by a thin steel baffler.

Molten salt forming the lower pool was LiF-NaF-ZrF4 with the melting temperature of 558 ^{o}C, while for the upper pool the composition LiF-NaF-KF with melting temperature of 454 ^{o}C was used. The difference in the melting points of both salts was 104 ^{o}C large enough to allow simulation of heat transfer peculiarities in the stratified system under conditions corresponding to reactor.

The objectives of tests were as follows:

- Simulation of the focusing effect of the heat flux when the heating of the upper layer is due to the convective heat transfer from the bottom pool. For these cases, the situation with and without top crust is considered. For the first case, the convection pattern in the upper layer is uncoupled with the convection in the lower layer. The second case presents coupled convection in both layers.
- Study of the focusing effect as a function of dimensionless numbers such as Biot (Bi) and Nusselt (Nu_{up}, Nu_{sd}) numbers.
- Verification of correlations for upward and downward heat transfer under variable conditions at the top pool surface from isothermal to almost adiabatic.

This paper contains results of post-test numerical calculations for the MASCA Project and their analysis.

2. The description of numerical model

For numerical simulation of heat exchange in the stratified “corium-metal” system the numerical model was used, where the flows of a heat-generating viscous fluid in a field of gravity force are considered utilizing Boussinesq approximation. The flows are described by the conservation equations of mass, movement and energy.

The equation of mass conservation (the continuity equation) is

$$\mathrm{div}\,\mathbf{v} = 0, \quad \mathbf{x} \in \Omega, \quad t > 0. \tag{3.1}$$

Here $\mathbf{v} = (v_1, v_2, v_3)$ is the velocity, t is the time. The flow is considered in the simple calculated domain:

$$\Omega = \{\mathbf{x} \mid \mathbf{x} = (x_1, x_2, x_3), \quad 0 < x_1 < L, \quad 0 < x_2 < D, \quad 0 < x_3 < H\}.$$

The momentum equation in the Boussinesq approximation for buoyancy force can be written in the form:

$$\frac{\partial \mathbf{v}}{\partial t} + C(\mathbf{v})\mathbf{v} + \mathrm{grad}\, p - \nu\, \mathrm{div}\,\mathrm{grad}\mathbf{v} = \beta g \mathbf{e}(T - T_\omega), \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{3.2}$$

where p is the pressure normalised to the density, ν is the kinematic viscosity, β is the thermal expansion coefficient, g is gravitational acceleration, $\mathbf{e} = (0,0,-1)$, is the unit vector for defining the gravity force, T is the temperature, T_ω is the temperature at the upper and lower bounds of parallelepiped.

The energy equation with uniform volumetric energy sources has the form

$$\frac{\partial T}{\partial t} + C(\mathbf{v})T - a\, \mathrm{div}\,\mathrm{grad}\, T = \frac{q}{c\rho}, \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{3.3}$$

where $a = k / (c\rho)$ is the thermal diffusivity, k is the thermal conductivity, c is the specific heat and ρ is the density. The quantity q is the power of uniform volumetric heat generation.

The calculations were carried out on a basis of the two-dimensional approach, in which the side-wall heating in slice-geometry was replaced by equivalent volumetric heating for power corresponding to experimental data.

For modeling of stratification, the some changes were made in CONV code, which have permitted to set various properties for upper and lower layers. The boundaries of layers were fixed. The additional immovable layer with the finite thermal conductivity settled down between fluid layers and simulated a baffler used in experiments. On upper boundary, a fixed layer was disposed also, which simulated the upper restrictive plate, used in experiment. Moreover, the opportunity of redistribution of volumetric heat rate and additional correction of thermal conductivity coefficients was stipulated depending on a layer in which given point lies. The block of formation of boundary conditions for setting an internal boundary condition on boundary betwen layers and condition of reradiation on the upper boundary was modified.

The heat flux on the upper boundary is considered as $q = \sigma\varepsilon_{eff}\,(T^4 - T^4_{sur})$, where T is local temperature of a salt surface, T_{sur} is average temperature of lower surface of a heat exchanger and vertical surfaces of a bath above level of fluid salt, ε_{eff} is effective radiant emittance calculated as

$$\varepsilon^{-1}_{eff} = \varepsilon^{-1}_{salt} + S_{salt}/S_{sur}\ (\varepsilon^{-1}_{st} - 1),$$

where ε_{salt} and ε_{st} – radiant emittances of salt and steel, $S_{salt} = 2RZ$ and $S_{sur} = 2RZ + 2(2R + Z)H$ – surface of molten salt and surrounding surface (Z – width of bath, H – distance from surface of molten salt to the upper heat exchanger.

For conducting of calculations the new effective difference schemes for solving of the unstable Navier-Stokes equations in primitive variables such as velocity and pressure [1] were used. A feature of these schemes is special approximation of the differential operators. This approximation allows to obtaining difference operators that inherit fundamental properties of the corresponding initial differential operators. The operators that approximate the viscous terms are self-consistent and positive. They provide the dissipation of kinetic energy.

The details of testing of developed model and computing algorithm of its solution can be found in [2]. The numerical code used for calculations represents the CONV code [1] in multiblock implementation and includes above model and new effective difference schemes for solving of the unstable Navier-Stokes equations in a primitive variables.

The outcomes of modeling of stratification by means of the modified CONV code are submitted below.

3. Calculated results

3.1 Test matrix

The test matrix includes 17 different steady state regimes of convection. To get different regimes the following parameters were varied: heating power of the lower pool, cooling salt temperature, temperature of the upper heat exchange.

The investigated regimes differ by presence of crust on both side and upper boundary of the upper layer and upper and lower boundaries of lower pool, and also by the temperature relation of lateral surface of the upper layer (T_{sd}) and surface above this layer (T_{sur}).

The matrix of test regimes is shown in Table 1, which presents existence of crust at cooled surfaces and interface between lower and upper salt pools.

All regimes, indicated in table 1, were simulated by means of CONV code.

Table 1: Experimental regimes studied in the test series.

Reg#	Qin, W	Tsd, C	Tsur, C	Lower pool crust		Upper pool crust	
				Top	Bottom	Top	Side
1	852.83	620	543	N	N	N	N
2	1767.6	597	503	N	N	N	N
3	1825.0	555	448	N	Partial	N	N
4	1142.3	529	422	N	Y	N	N
5	1096.8	483	347	Y	Y	N	N
6	894.3	430	313	Y	Y	Y	Y
7	819.87	436	305	Y	Y	Y	Y
8	1221.92	372	245	Y	Y	Y	Y
9	1211.49	374	307	Y	Y	Y	Y
10	1807.91	401	261	Y	Y	N	Y
11	1970.32	413	381	Y	Y	N	Y
12	2313.30	431	449	Y	Y	N	Y
13	2926.94	455	477	Y	Y	N	Y
14	4565.0	500	525	N	Y	N	N
15	3939.15	446	487	Y	Y	N	Y
16	3636.89	422	233	Y	Y	N	Y
17	5060.46	433	295	N	Y	N	N

3.2 Convection regime in the lower pool

The experiments were carried out in a wide range of characteristic parameters, such as modified Rayleigh number (Ra ') under conditions of crust formation both on the vessel simulating a sidewall and on the upper boundary. The convection regimes without crust and with crust on the lateral and upper boundaries of lower pool were realized. The regimes with crusts are prototypic from the point of view reactor applications. In fig. 1, 2, 3 two-dimensional temperature fields are submitted in the lower pool and in the upper layer as isotherms in a range from 723 up to 823K for 7, 10 and 16 regimes, accordingly (all regimes with crusts on both boundaries).

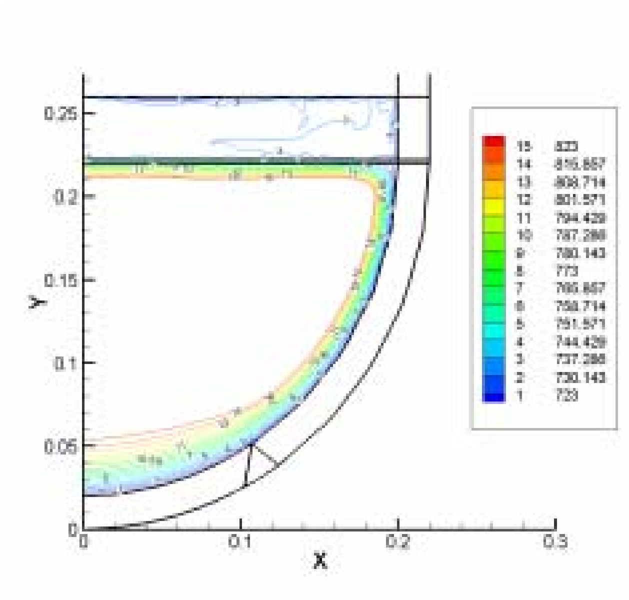

Fig. 1: Isotherms in the range from 723 to 823 K for 7 regime.

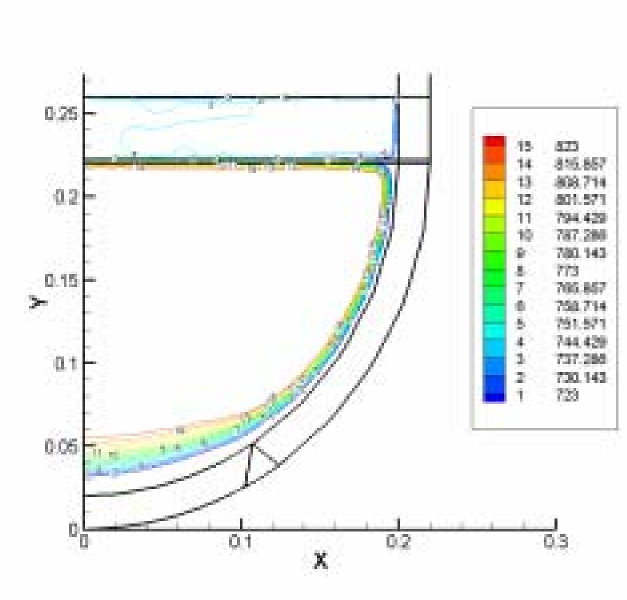

Fig. 2: Isotherms in the range from 723 to 823 K for 10 regime.

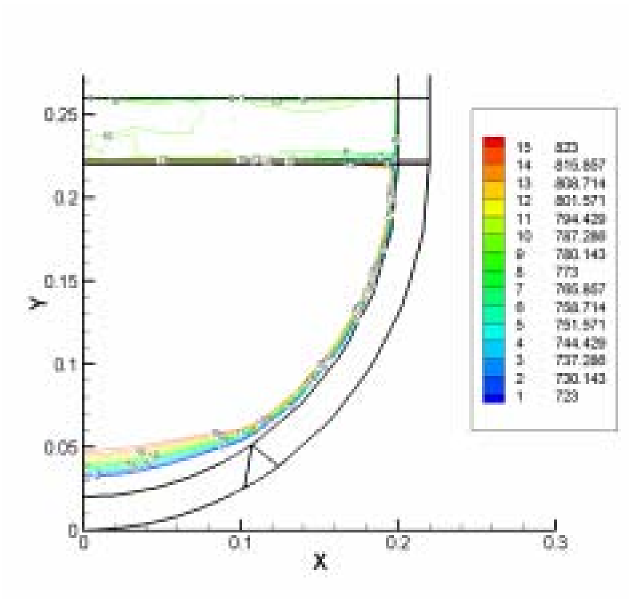

Fig. 3: Isotherms in the range from 723 to 823 K for 16 regime.

In the figures 4, 5, 6 the calculated vertical distributions of temperature of salt in lower heated volume are shown, including crust on the upper boundary and boundary layer. The calculated data concern the same regimes, #7, 10, 16. Together with calculated data the experimental ones are also presented. Fig. 4, 5, 6 demonstrate satisfactory correspondence of the calculated data to experiments. The especially good correspondence takes place for the upper part of a bath. The divergence is observed in the lower part, in crust area on the lower part of test-wall. The comparison of temperature profiles in fig. 4 - 6 shows, that the calculated crust thickness appears approximately in 1.5 times less actually measured. One of reasons of divergences can consist in heterogeneity of crust thickness across the bath. The experiments show, that the crust thickness is maximum in the central section of the bath and much less near to side (heated) walls of the bath. The measurements of vertical temperature profile in the given experiment were carried out in the central section of the bath, where the crust thickness is maximum. In used two-dimensional model all salt parameters, including crust thickness, were considered completely homogeneous across the bath. The other reason of divergences can be that in calculations a volumetric heat generation inside of the crusts is considered to be the same as in a liquid part of the lower salt. Actually, in experiment with sidewall heating the conditions of the crust heating due to inhomogeneous crust thickness should differ from conditions of a liquid heating.

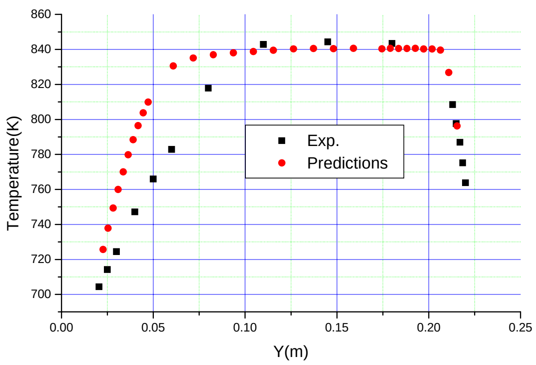

Fig. 4. Vertical temperature profile in the central section of the lower pool, regime 7.

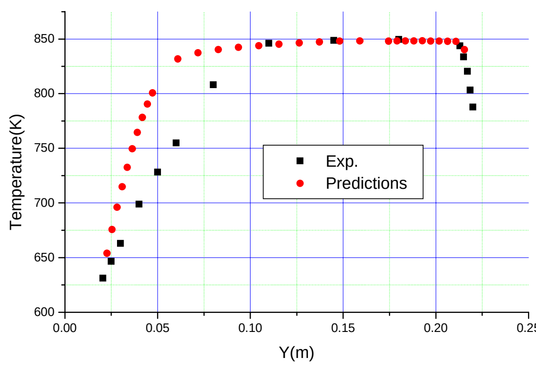

Fig. 5. Vertical temperature profile in the central section of the lower pool, regime 10.

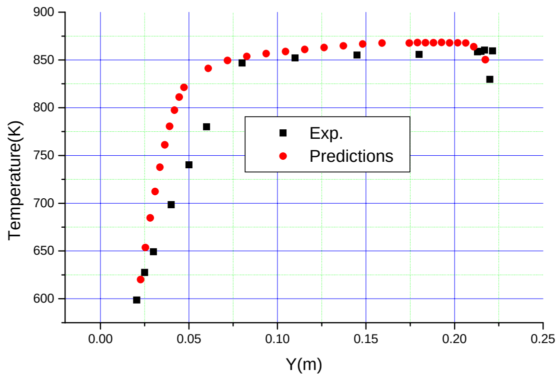

Fig. 6. Vertical temperature profile in the central section of the lower pool, regime 16.

The numerical investigations the partitioning of heat flux on the upper and side boundaries of the lower salt (the corium models) show, that the separation of total heat generated in lower volume, happens as follows.

For isothermal conditions, when crusts are present both on lower and on the upper boundaries, the partitioning of total heat generated in the pool corresponds about 55% for upward heat transfer, that with a good accuracy is in accordance with the experimental data and is rather close to the Mayinger's correlations.

Without crust on the upper surface the calculated partitioning values decrease and appear to be approximately in 1.5 times below then experimental ones, though the calculated temperature on a upper boundary of lower pool in all regimes appears to be a little bit less then measured one (see fig. 7 - 12).

3.3. Convection in the upper pool.

Figures 7 - 9, 10 - 12 represent the calculated data concerning to heat transfer in the upper layer.

In figures 7, 9, 11 the horizontal (radial) distributions of temperature on upper boundary of the upper layer are shown. It is visible from figures, the calculation rather well reproduces experimental data. The numerical predictions regularly give somewhat underestimated values of temperature near the central section of the bath. On a rim the calculated and measured temperatures coincide with an exactitude of 5 degrees.

Figures 8, 10, 12 are demonstrated radial distributions of temperature on the lower boundary of the upper layer. The comparison to experimental data reproduced in the same figures, shows the good consent of outcomes with an exactitude 5 - 10 degrees.

The table 2 submits calculated and experimental data on distribution of heat flux from the upper layer to top and in side boundaries and focusing effect. Qin is total power entered in the lower pool, Qdn is the heat flux coming to the upper layer from lower heated volume, Qup is heat flux on the upper boundary in the upper layer.

Table 2. Experimental data vs numerical predictions for heat fluxes through the lower and upper boundaries in the upper layer and focusing-effect.

Reg#	Qup/Qdn (exp)	Qup/Qdn (calc)	Focusing (exp)	Focusing (calc)
1	0.842	0.814	0.74	0.92
2	0.691	0.800	1.47	1.4
3	0.698	0.818	1.44	1.37
4	0.736	0.870	1.26	1.19
5	0.696	0.853	1.45	1.38
6	0.751	0.792	1.22	1.04
7	0.782	0.786	1.03	1.06
8	0.728	0.735	1.29	1.32
9	0.691	0.687	1.47	1.42
10	0.578	0.661	2	1.69
11	0.434	0.432	2.7	2.83
12	0.218	0.224	3.72	3.87
13	0.143	0.255	4.1	3.70
14	0.094	0.247	4.31	3.76
15	0.183	0.176	3.89	4.11
16	0.472	0.480	2.66	2.6
17	0.917	0.647	3.2	1.78

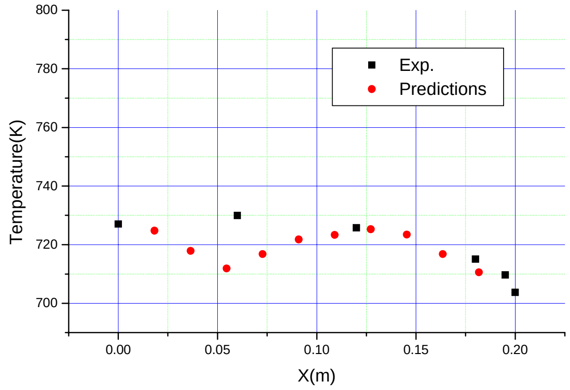

Fig. 7. Temperature distribution vs radius at the upper boundary in the upper pool for regime 7.

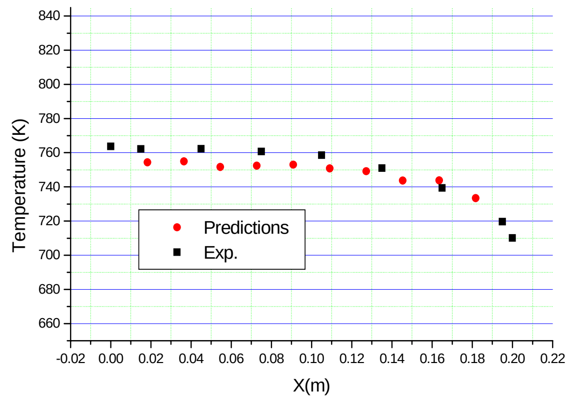

Fig. 8. Temperature distribution vs radius at the lower boundary in the upper pool for regime 7.

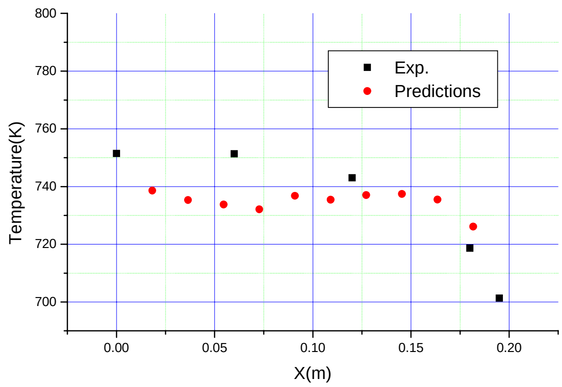

Fig. 9. Temperature distribution vs radius at the upper boundary in the upper pool for regime 10.

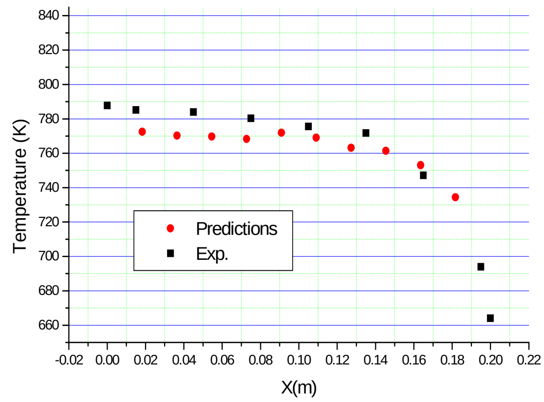

Fig. 10. Temperature distribution vs radius at the lower boundary in the upper pool for regime 10.

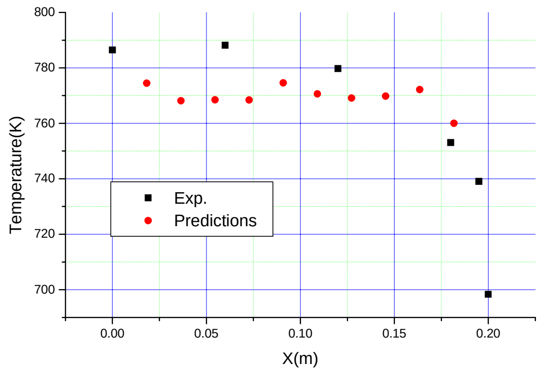

Fig. 11. Temperature distribution vs radius at the upper boundary in the upper pool for regime 16.

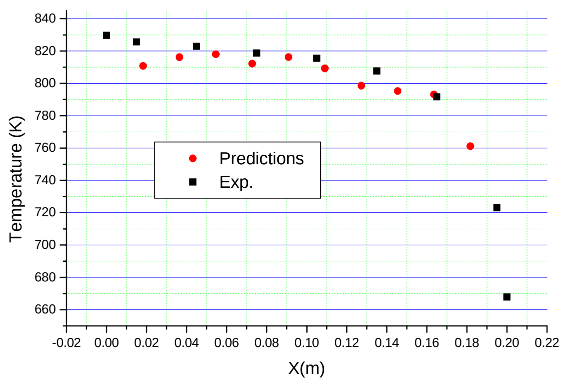

Fig. 12. Temperature distribution vs radius at the lower boundary in the upper pool for regime 16.

At last, in figure 13 the comparison of numerical predictions of focusing-effect with experiments and data obtained with the 0-D model [3] is given.

From table 2 and figure 13 one can see that two-dimensional hydrodynamic calculation satisfactorily describes of heat transfer regime in the upper layer.

In a series of cases 0-D the model gives the best correspondence with experimental data, than two-dimensional calculations.

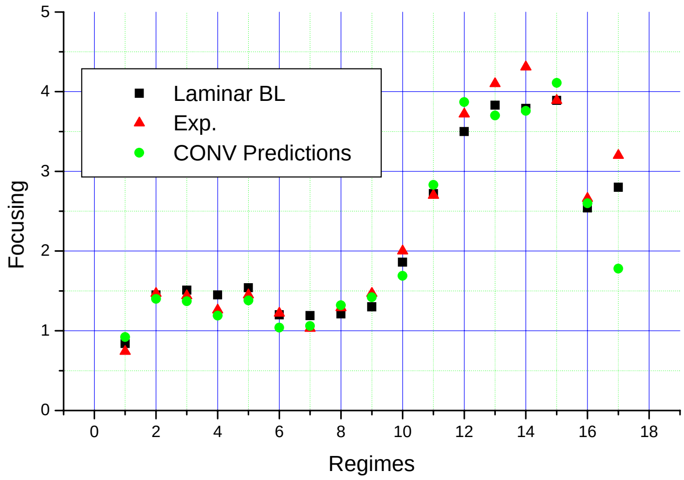

Fig. 13. Comparison focusing effect of heat flux for a vertical boundary layer: measured, calculated on the base of 0D model and predicted by CONV code.

The maximal difference of 2D numerical predictions from experimental data on focusing-effect is observed in conditions without crusts in the upper layer and without crusts or with partial ones in the lower pool. In cases with crusts both on side and upper boundaries of the upper layer 2D outcomes are close to experiment.

The obtained results allow to speak about adequate modeling of heat transfer phenomenon in stratified liquid pool with 2-D CONV code..

4. Conclusions

For numerical simulation of the heat and mass transfer processes in stratified volume the model of two liquids divided geometrically and having different thermal-physical properties and volumetric heat generation was developed and included into CONV code. The salt experiments within the framework of the MASCA Project were simulated by means of this model.

In accordance with the test matrix 17 steady state regimes of convection were studied.

These regimes were performed in a broad range of characteristic parameters (as Ra’ number, presence of the crusts on boundaries of the upper and lower volumes, conditions of radiative heat exchange with top surface). The boundary conditions on the top surface of the pool varied from isothermal to almost adiabatic. In all cases the reasonable concurrence to experimental data is obtained.

Heat transfer in the lower pool was found to be rather close to the correlations of Mayinger [4], which were obtained in similar range of Rayleigh numbers.

Obtained data on the heat transfer were analyzed and compared to the 0D model. Both models give reasonable concurrence to experimental data.

References

1. Aksenova A.E., Chudanov V.V., Pervichko V.A., Semenov V.N. Strizhov V.F. // Development and application of the CONV Codes. // In Proc. RASPLAV Seminar 2000, Munich, November 2000. CD-disk.. Session 3: Theoretical analysis. 18p.
2. Chudanov V.V., Aksenova A.E., Pervichko V.A. // Development of 3D unified computational tools to thermalhydraulic problems. Proc. 10-th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-10) Seoul, Korea, October 5-9, 2003. (CD-disk, paper E00003.pdf).
3. V.G. Asmolov, S.S. Abalin, A.I.Surenkov, I.P. Gnidoy, B.V. Barkovsky, N.V. Komissarova, D.Yu. Chuvilin, Yu.V. Rybakov, V.F. Strizhov, V.N. Semenov. Study of thermal hydraulic processes in a stratified molten pool. **MP-TR-13,** December 2003.
4. Mayinger, F., Jahn, M., Reineke, H. and Steinbrenner, V., 1976, “Examination of Thermohydraulic Processes and Heat Transfer in a core Melt”, BMFT RS 48/1. Institute fur Vrefanhrenstechnic der T.U., Hanover, Germany.