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Modelling of Reactor Core Behaviour under Severe Accident Conditions. Melt Formation, Relocation and Evolution of Molten Pool

Current status

Presented by

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March 6-8, 2007

Drezden, Germany

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- In order to describe melt behavior in the late stage of core degradation, the 3D unified thermal hydraulic technique for simulation of heat and mass transfer processes in complex domains was developed in the CONV code:
  - The model for calculation of flows with a variable density without the Boussinesq approximation was developed in the CONV code. The necessary modification of the numerical algorithm to fast solving of the pressure correction equation with use of the algebraic solver on the basis of Fast Fourier Transformation (FFT) and verification of the software were carried out. Comparison with Boussinesq model against such parameters as 3d heat flux distribution on the lower head and possible crust formation depending on the power density and the external cooling were conducted. Verification of the modified software is carried out against such experiments as RASPLAV and SIMECO [S1].

[S1] *Seghal B.R. et al. Experiments on the effects of melt pool stratification on vessel thermal loads in SIMECO facility.*

Development of the three-dimensional CFD code

Incompressible media

Navier-Stokes equations in primitive variables within Boussinesq approximation for buoyancy together with convection/diffusion equation for the temperature are used for modeling thermal and hydrodynamics flows:

$$\frac{d\mathrm{v}}{dt} = -\frac{1}{\rho_0}\, grad\, p + div\left(\frac{\nu}{\rho_0}\, grad\, \vec{\mathrm{v}}\right) + \beta g \Delta T$$

$$div\, \vec{\mathrm{v}} = 0$$

$$\frac{d\rho_0 C_v T}{dt} = div\left(\chi\, grad\, T\right) + q$$

Problem with a variable density

Navier-Stokes equations with variable density are applied.

Numerical implementation of the operator splitting scheme :

a fast solver for pressure correction equation, based on Modified Preconditioned Richardson Method with Fast Fourier Transformation (FFT) .

$$\frac{d\rho\mathrm{v}}{dt} = -grad\ p + div\left(\mu\ grad\ \vec{\mathrm{v}}\right) + g$$

$$div\ \vec{\mathrm{v}} = 0$$

$$\frac{d\rho C_v T}{dt} = div\left(\chi\ grad\ T\right) + q$$

Modified Preconditioned Richardson Method with Fast Fourier Transformation (FFT)

<u>Pressure correction equation:</u>

$$\mathrm{div}_h\left(\frac{1}{\xi}\,\mathrm{grad}_h\, p_\varepsilon^{n+1}\right) = \frac{1}{\xi}\,\mathrm{div}_h\, \mathrm{v}_\varepsilon^{n+1/2}$$

Maximum of convergence velocity is reached under

$$\alpha = \alpha^* = \frac{2}{\eta_{\min} + \eta_{\max}}$$

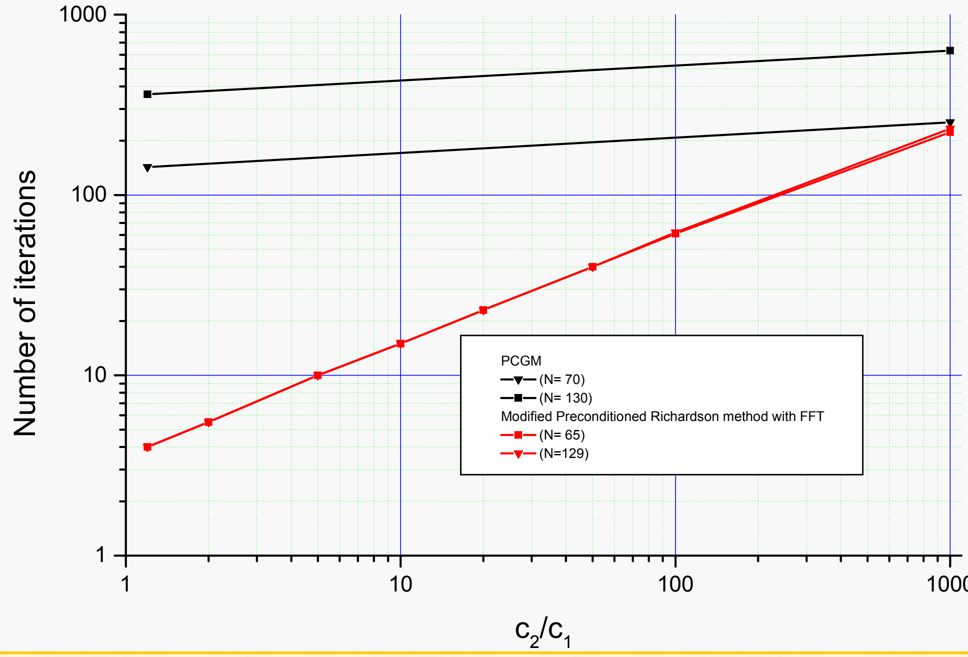
Iteration algorithm for matrix A:

$$A^T = A > 0$$

$$P(x^{k+1} - x^k) = \alpha r^k,\; k \in N$$

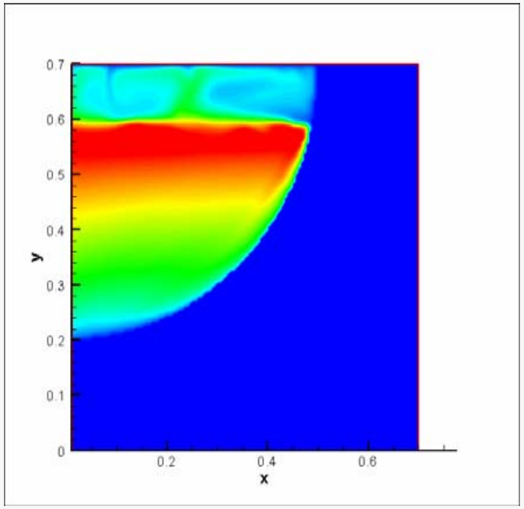
$$r^0 := b - Ax^0$$

$$\begin{cases} Pz^k := r^k \\ x^{k+1} := x^k + \alpha z^k \\ r^{k+1} := r^k - \alpha A z^k \end{cases}$$



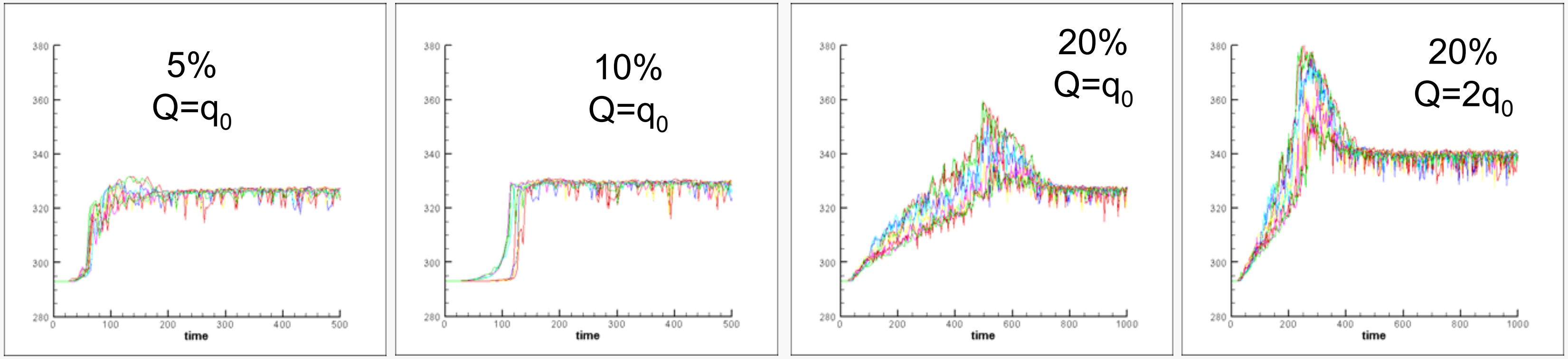
Inversion of Stratified Liquid Layers

Analysis of SIMECO tests



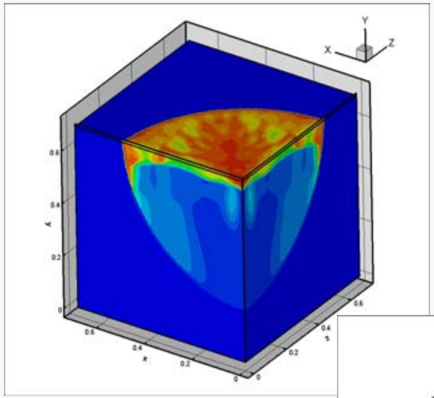
- The rate of mass transport between compositional different layers is defined by the bulk Richardson number: $Ri=gH\Delta\rho/\rho V^2$
- The velocity scale in a convective layer can be written as $V^2=\beta\Delta TgH$, which implies that $Ri=(\Delta\rho/\rho)/(\beta\Delta T)$.
- A mixing time scale of two layers can be defined as $t_{mix} \sim (\Delta\rho HC_p)/(\alpha\beta q)$
- Presented numerical predictions qualitatively coincide with experimental data from the SIMECO facility [S1].

Temperature history in the upper layer



3D inversion at the different percentage densities ratio, t=t0

5%



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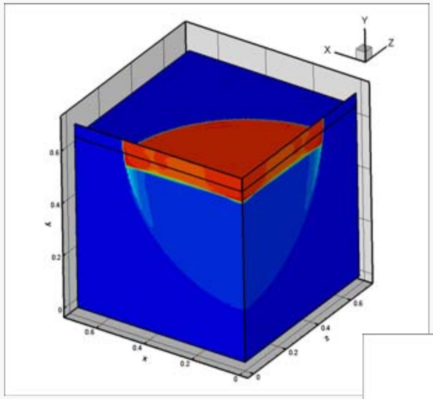

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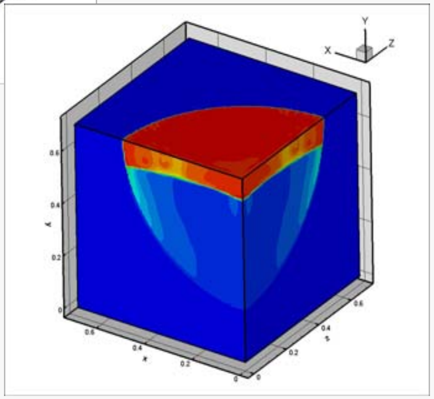

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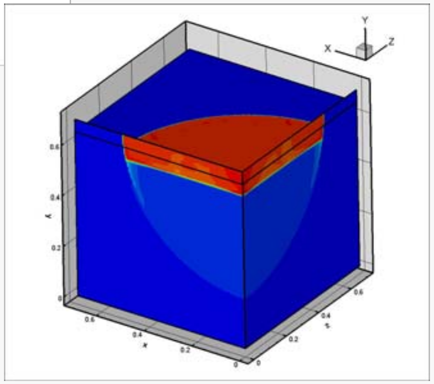

As a result of heating 3D hemispherical field an instability on boundary of cold and hot layers occurs. 3D plums are formed. That gives earlier inverse in comparison with relevant 2D axial and 3D flat geometries at the small aspect ratios.

- The numerical simulation of natural convection and heat flux distribution was supplemented with the theoretical analysis of major phenomena such as boundary layers formation, with the analysis of energy balance in a heat generating fluids.
- Theoretical dependences were compared with the results of calculations, namely for such processes as:
  - free convection in a heat–generating fluid for cylindrical geometry;
  - convective heat exchange for a heat-generating fluid in a upper of enclosure.

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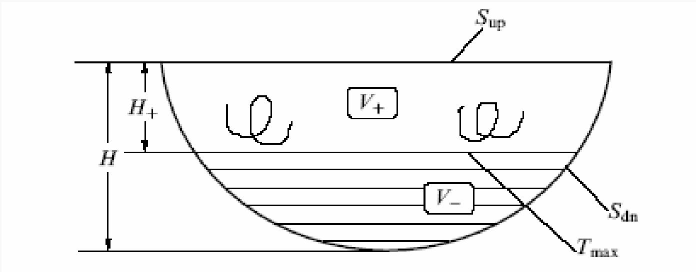
- Heat generating fluids exhibit temperature stratification depending upon boundary conditions on the top (isothermal or adiabatic). Corresponding theoretical assessments for the heat transfer and their dependence upon dimensionless parameters such as Rayleigh number were compared with numerical results.

[B1] *L.A. Bolshov, P.S. Kondratenko, V.F. Strizhov*, A semi-quantitative theory of convective heat transfer in a heat generating fluid, Int. J. Heat and Mass Transfer, Vol.41 (1997), № 10, pp.1223-1227.

[B2] *L.A. Bolshov, P.S. Kondratenko,* Limiting angular characteristics of heat transfer and stratification in a heat-generating fluid, International Journal of Heat and Mass Transfer, Vol.43 (2000), № 20, pp.3897-3905

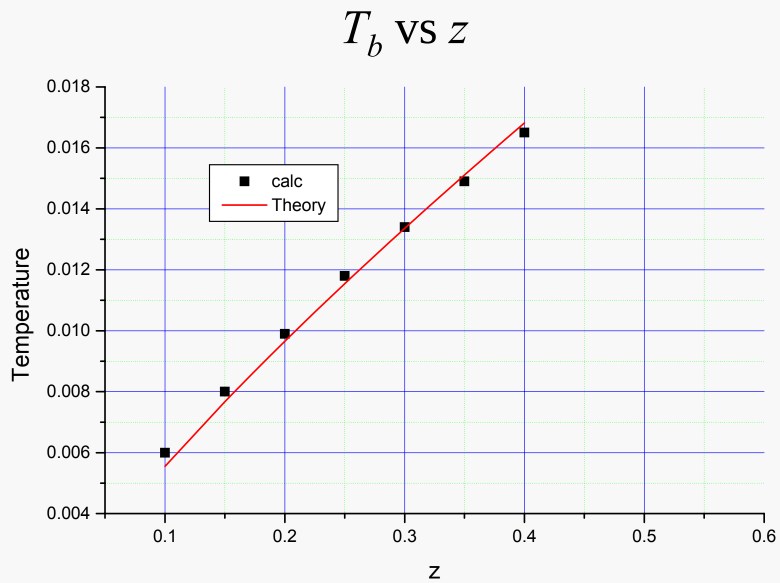
[B3] *L.A. Bolshov, P.S. Kondratenko, V.F. Strizhov*. Buoyancy-induced convection of heat generating liquid. Uspehi Fiz. Nauk Vol.171(2001), №10, pp.1051-1070

Heat exchange features of a heat generating fluid in prototypical volume



The central vertical slit occupied by a volume with fluid: S_{up} and S_{dn} the upper horizontal and lower boundaries, correspondingly; T_{max} – horizontal plane, taking place through a point of a maximum value of temperature in volume; V_+ and V_- - domains of volume located above and lower of a plane T_{max}; H- vertical size (height) of all volume; H_+ - height of domain V_+.

T_b vs z



Analytical evaluation for heat flux q on the boundary and temperature distribution T_b in basic volume for laminar boundary layer (BL) at $\theta^* << \theta << 1$ and $\delta << z << R$ [B3]

$$q \propto \theta^2 \quad T_b \propto \left(\frac{z}{H}\right)^{4/5}; \quad \theta_*^2 \sim \frac{\delta(\theta_*)}{R}$$

z – coordinate, counted from a pole level (θ=0) on a vertical upwards, R – radius of a boundary curvature, δ – thicknesses of BL.

Heat fluxes in BL demonstrate a dependence close to square-law: $q \sim a + b\theta^2$ in correspondence with theoretical analysis [B2]. This result were submitted on 9th Meeting CEG-CM in Paris, in March 7-9, 2006.

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Free convection of a heat generating fluid in a quasi two-dimensional geometry

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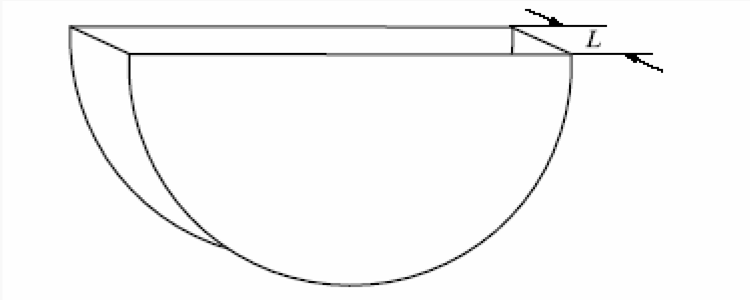
Analytical evaluation



$$L << R$$

Maximum correspondence of a heat transfer in quasi two-dimensional volume to prototipical volume is reached under condition [B3]

$$\frac{L}{R} >> \mathrm{Ra}_i^{-1/6}$$

L- thickness of vertical section,
R – curvature radius,
Ra_i – modified Rayleigh number.

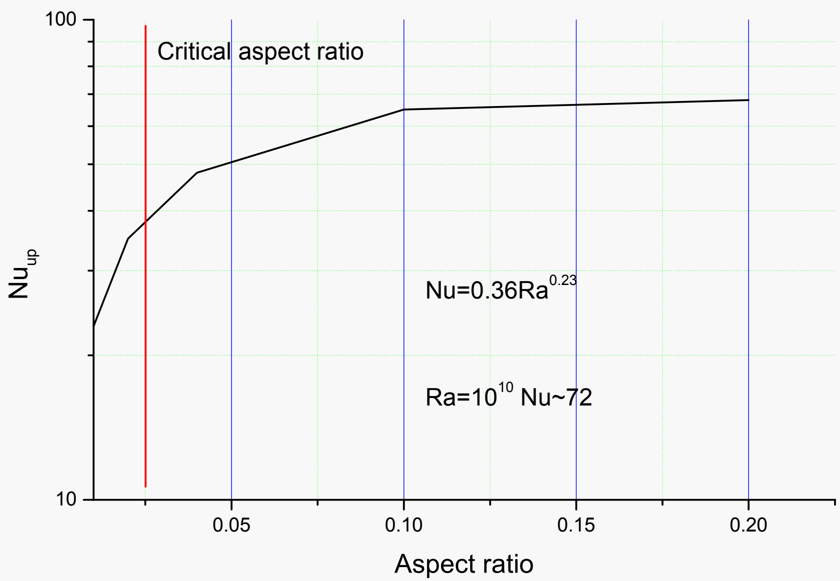
Numerical predictions

Critical aspect ratio for $\mathrm{Ra} = 10^{10}$

$$\frac{L}{R}(\mathrm{Ra} = 10^{10}) \approx 0.025$$

Nusselt number in this case

$$\mathrm{Nu}(\mathrm{Ra} = 10^{10}) = 0.36\mathrm{Ra}^{0.23} \approx 72$$



Convective of a cooling down fluid without interior heat sources

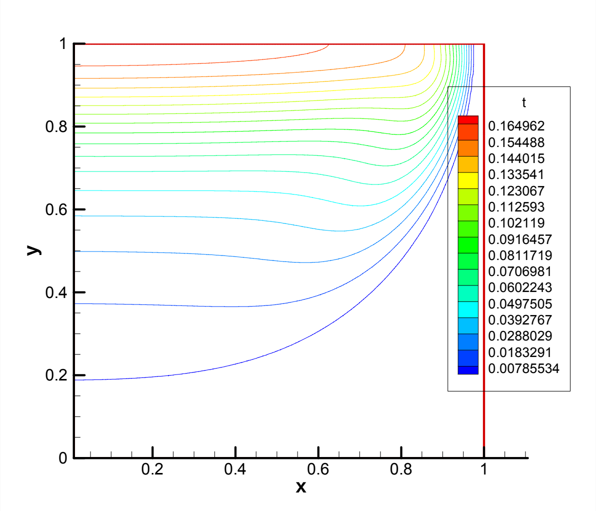
Analytical evaluation

Temperature distribution in internal volume [B3] $T_b(z,t) = T_0(t)\exp\left(k\frac{z}{R}\right)$

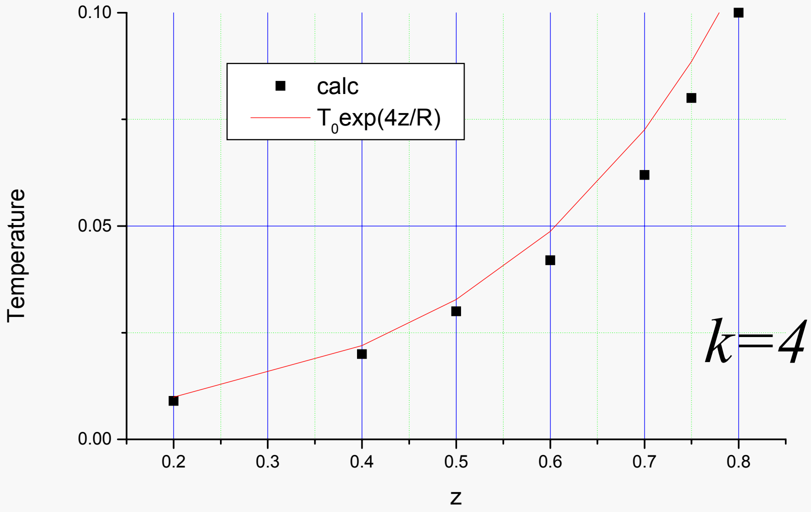
T_0- temperature value, counted form the temperature on the boundary, z – coordinate, counted from a pole level (θ = 0) on a vertical upwards, R – radius of a boundary curvature, t – time, k – dimensionless value.

Numerical predictions

Temperature filed



T_b vs z



Convective of a cooling down fluid without interior heat sources (#2)

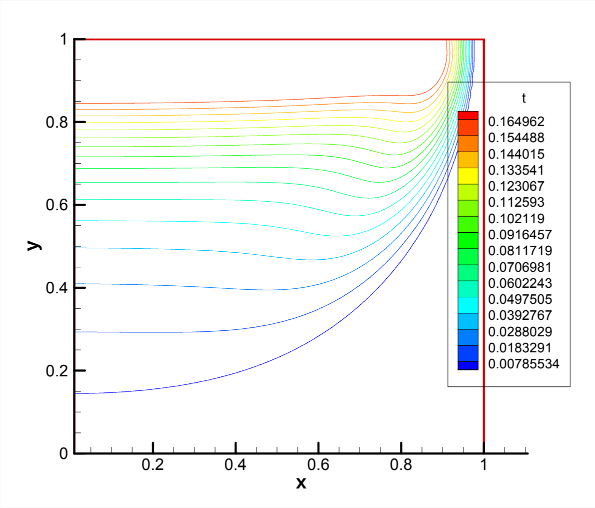
Analytical evaluation

Heat flux density distribution on a boundary [B3] $q(\theta,t)=q_{\min}(t)\exp\left(p\theta^2\right)$

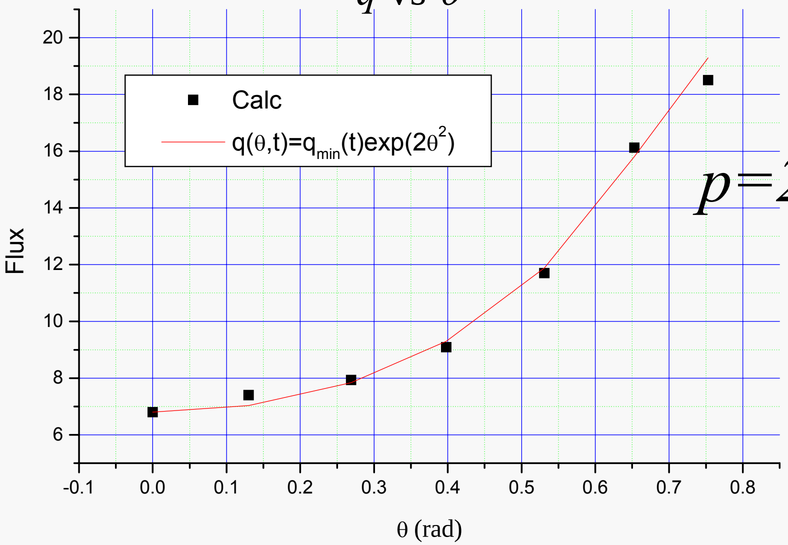
θ - angle, q_{min}- minimum value of heat flux density on boundary realized under θ=0, t - time, p – dimensionless parameter.

Numerical predictions

Temperature filed



q vs θ



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- The adaptation of the improved three-dimensional CONV code was carried out for conditions of the LIVE tests (Fluhrer et al., 2005), in order to simulate three-dimensional flows in the Boussinesq approximation for buoyancy on Cartesian grids with a local refinement near domain with singularities of flows. Algorithms, methods and software were validated against a wide class of experimental and benchmark tests: benchmark Davis, Jacob correlation, Benard convection, melting of pure gallium, Mayinger experiments for convection in a heat-generating fluid. The preliminary numerical simulation of circular heating used in experimental facility LIVE was carried out.

[F1] B.Fluhrer, H. Alsmeyer, A. Miassoedov et al. The experimental programme LIVE to investigate in-vessel core melt behaviour in the late phase. 2005

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Experimental Facility LIVE

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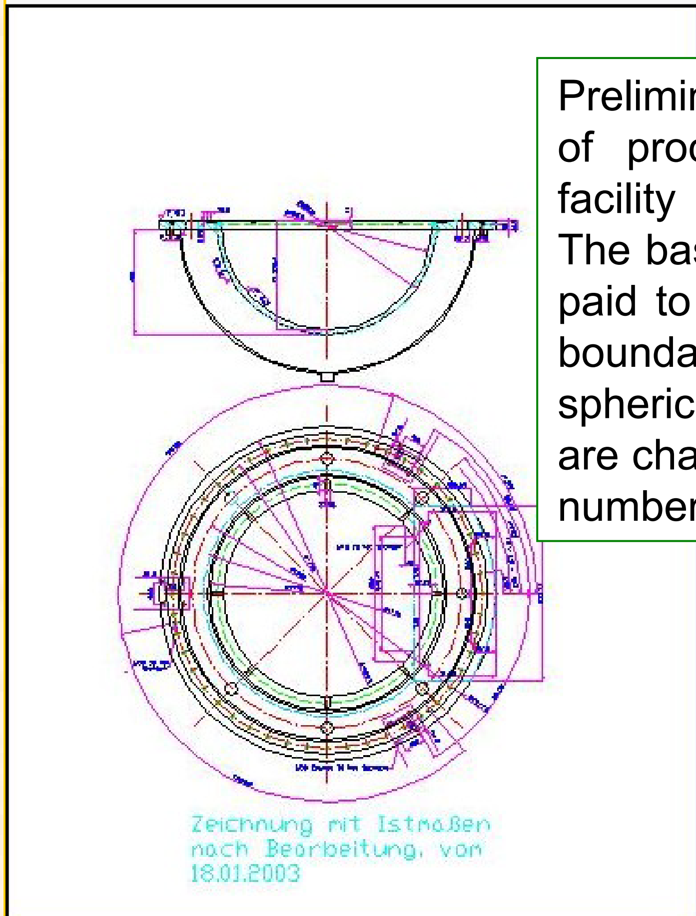
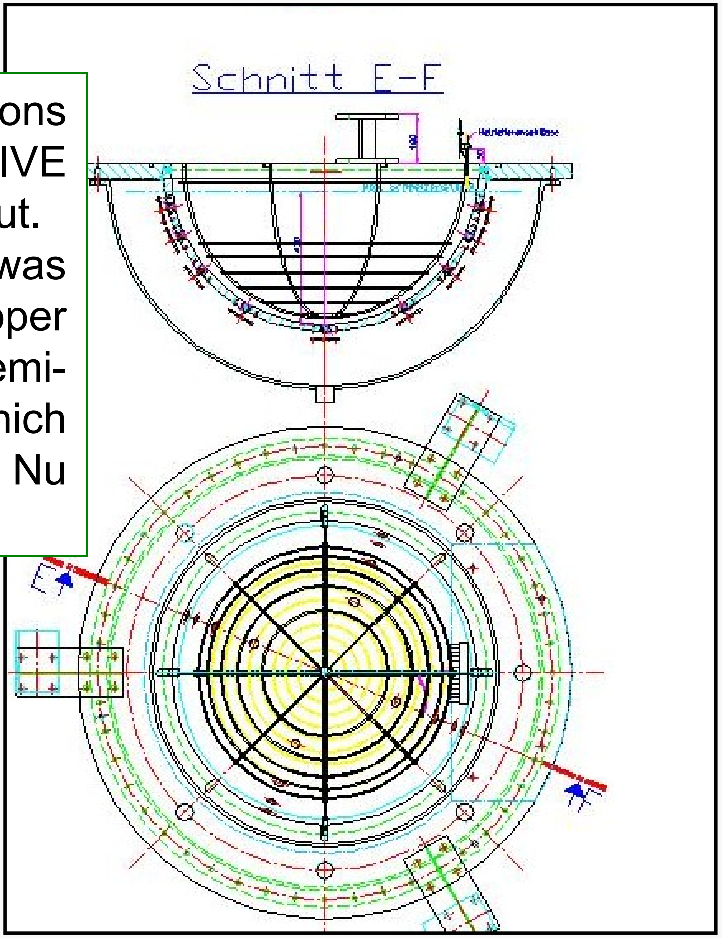
Dimensions



Preliminary calculations of processes in LIVE facility are carried out. The basic attention was paid to fluxes on upper boundary of hemi-spherical domain, which are characterized by Nu number.

Section E-F. Heater

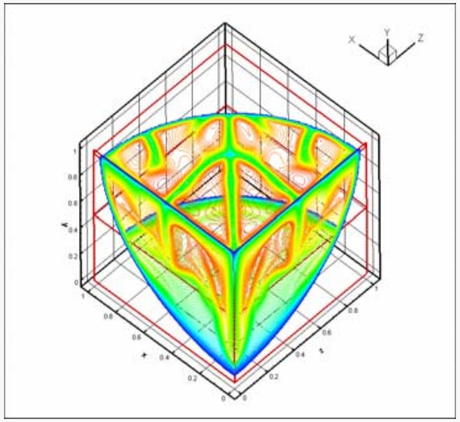


Analysis of Tests Performed under Similar to LIVE Conditions

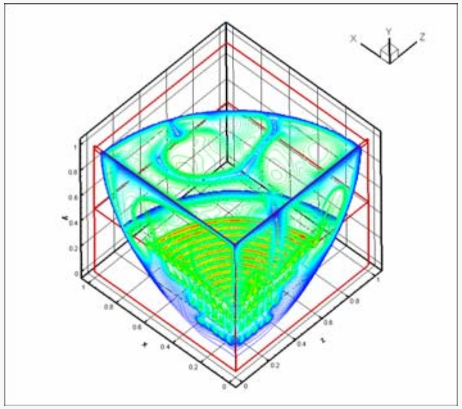
Comparison of uniform and circular heating

Uniform heat: $Ra=10^9$

3d temperature field

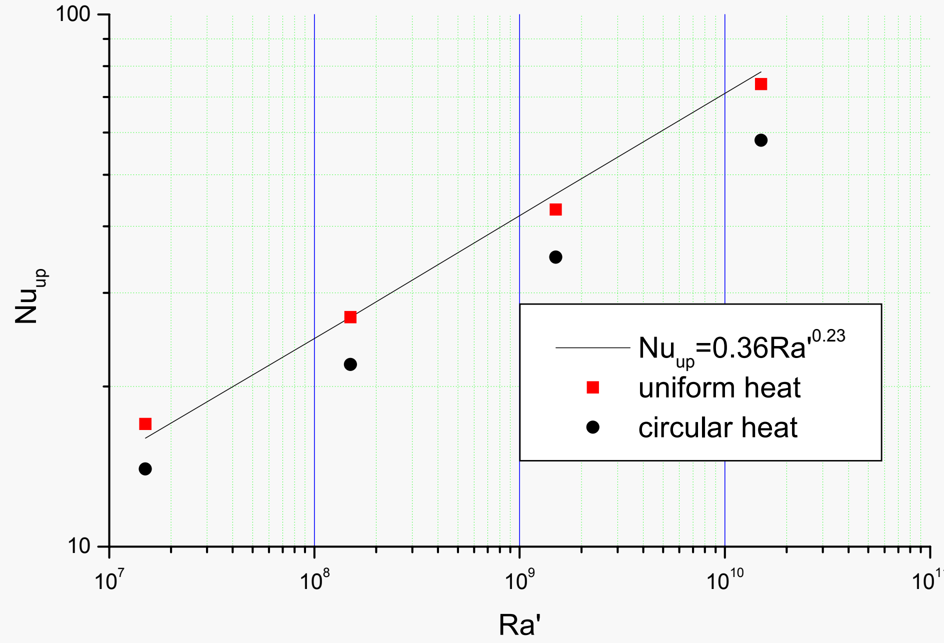


Circular heat: $Ra=10^9$



Nu vs Ra at different heating conditions

Comparison with correlations of M. Sonnenkalb (Proc. of Workshop on Large molten pool heat transfer, Grenoble, France, 1994)



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Preliminary LIVE calculations

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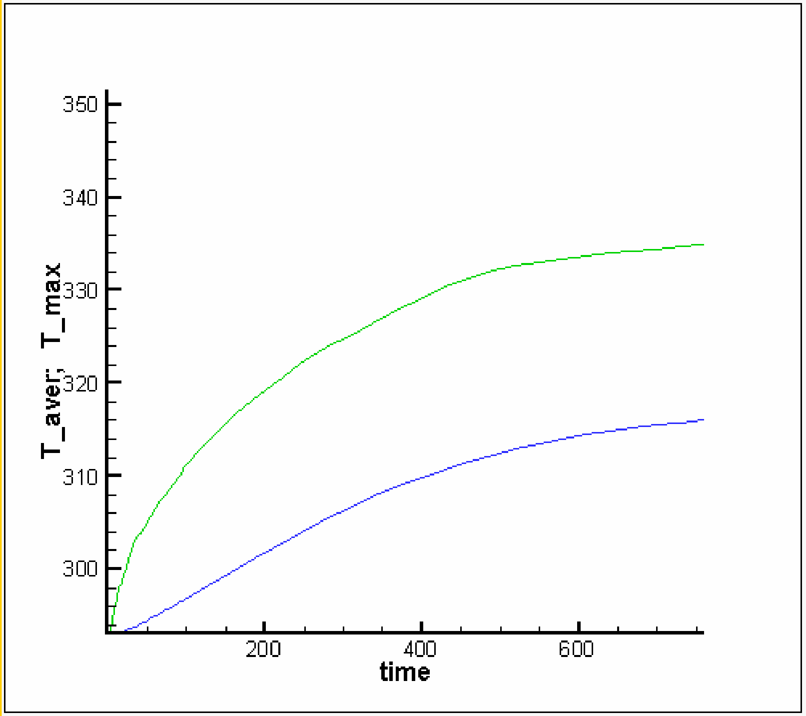
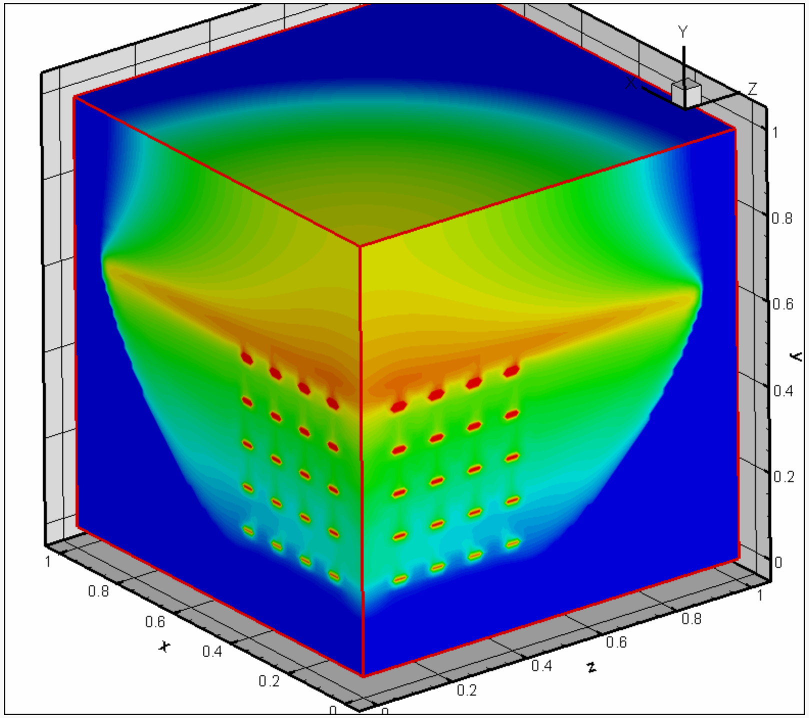
Adiabatic top boundary,
Isothermal side boundary, 273 K
Circular heating — 3 kW (in ¼ domain)

Melt level =0.7
Air level = 0.7÷1
3d hemispherical domain

Average and maximal temperatures



Isotherms



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Scope of Current Activities

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- According to the calendar plan for accounting period the following works on the task 10 are fulfilled:
  - The possibility of modeling of the melt flows simultaneously with a heat transfer in the reactor vessel and crust formation at high Rayleigh numbers is realized. The applicability of the realized approach is proved by the extensive validation against the results of molten-salt tests. It is concluded that the developed approach correctly predicts the absolute values of the crust thickness.
  - For modeling of phase transformations in binary alloys the numerical approach and computing module are developed, in which the (simplified) continuum model (Prakash&Voller, 1989) is used together with the original numerical algorithm for modeling of multiphase flows. Numerical predictions are successfully validated against the experimental data (Beckermann&Viskana, 1988) and numerical data (Lee&Tzong, 1995) for behavior of the water solute of chloride ammonium.
  - For simulation of turbulence flows was used the direct numerical simulation (DNS) approach and the developed algebraic turbulence model. For modeling of turbulence in 3D single-phase flows the Large Eddy Simulation approach is used. For modeling of turbulence in 3D two-phase flows the Direct Numerical Simulation (DNS) approach on sufficiently detailed grids and the original effective numerical methods for solving of CFD problems are used. The applicability of the developed turbulence approach was proved by the extensive validation against the 2D and 3D results of lid-driven flows (Ghia, 1982) and flows in tube (Toonder, 1997). In all the cases a good qualitative coincidence of numerical predictions with data is attained.

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Simulation of the melt flows simultaneously with a heat transfer and crust formation at high Ra

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- For testing the realized approach the data of salt experiments carried out on RASPLAV-Salt facility (see, for example, (*Chudanov, Proc. RASPLAV Seminar, Munich, 2000*) were used.
- The major findings from these tests:
  - crust thickness adjusts itself to the distribution of heat flux insignificantly changing it upon θ angle.
  - Within experimental errors, which were estimated as ±25% because of rather significant deviations from one to another test local distribution of the crust thickness is described by:

$$\frac{d(\theta)}{d_{max}(\theta=0)} = 1 - 4.44\cdot10^{-2}\theta + 2.22\cdot10^{-3}\theta^{2} - 3.65\cdot10^{-5}\theta^{3}$$

$$0^{o} \le \theta \le 41^{o}$$

(1)

$$\frac{d(\theta)}{d_{max}(\theta=0)} = 1.57 - 3.88\cdot10^{-2}\theta + 2.43\cdot10^{-4}\theta^{2}$$

$$41^{o} \le \theta \le 90^{o}$$

Simulation of the melt flows simultaneously with a heat transfer and crust formation at high Ra (#2)

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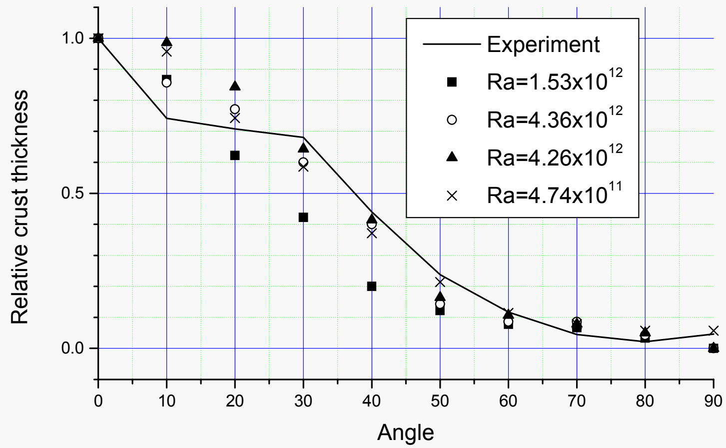
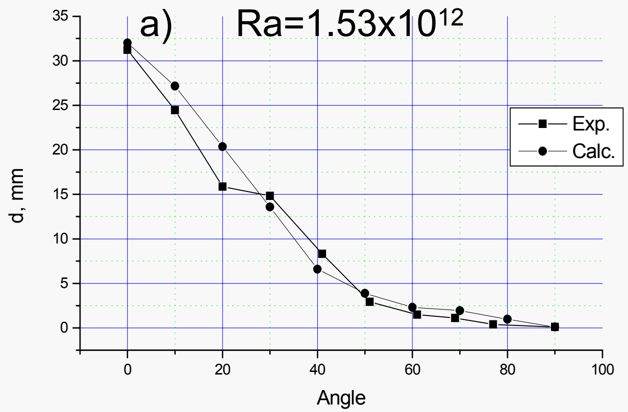
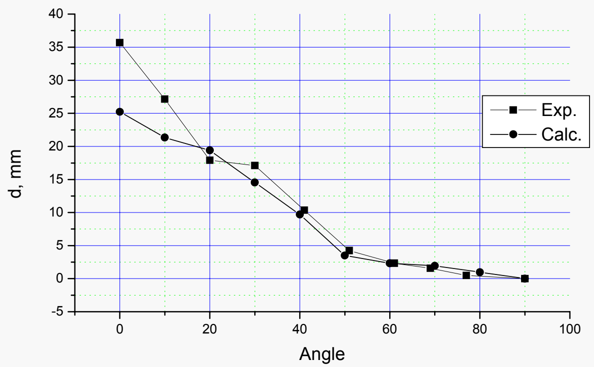
Local crust distribution



Crust thickness distribution along the inner surface of the test wall



b) Ra=4.36x10^12



Calculated values fit experimental data well. The greatest deviation is found in the bottom part of the pool where accuracy of evaluated in the tests heat fluxes is lower due to their lower values.
Summarizing all information presented above one may say that model predicts correctly the absolute values of the crust thickness.

Continuum mixture model

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C. Prakash, V. Voller, Numerical Heat Transfer, Part B, vol.15, 171-189, 1989.

$\rho_s = \rho_l = \rho \quad c_{pl} \neq c_{ps} \quad \mathbf{v}_s = 0$

Mass conservation

(A) $\nabla \mathbf{v} = 0,$

Momentum conservation

(B) $$\frac{\partial \mathbf{v}}{\partial t} + \nabla(\mathbf{vv}) = -\nabla P + \nabla(\nu_l \nabla \mathbf{v}) + g[\beta_T(T - T_0) + \beta_C(C - C_0)] - \frac{\nu_l}{K}\mathbf{v},$$

Energy equation

(C) $$\frac{\partial h}{\partial t} + \nabla(\mathbf{v}h) = -\nabla\left(\frac{k}{\bar{c}_p}\nabla T\right) + S_q,$$

Solute conservation

(D) $$\frac{\partial C}{\partial t} + \nabla(\mathbf{v}C) = \nabla(f_l D_l \nabla C) + S_C,$$

Enthalpy - temperature relations

(1) $h = \bar{c}_p T + f_l L$

Thermodynamic relations are obtained assuming local thermodynamic equilibrium. For phase diagram with straight liquidus and solidus lines

(2) $$f_l = 1 - \frac{1}{1-k_p}\frac{T - T_{liq}}{T - T_m}$$

(3) $$f_s = 1 - f_l$$

(4) $$C_l = \frac{C}{1 + (1 - f_l)(k_p - 1)}$$

(5) $$C_s = \frac{k_p C}{1 + (1 - f_l)(k_p - 1)}$$

(6) $$T_{liq} = T_m + (T_e - T_m)C / C_e$$

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Continuum mixture model (#2)

/Solidification of an Ammonium Chloride Water Solution/

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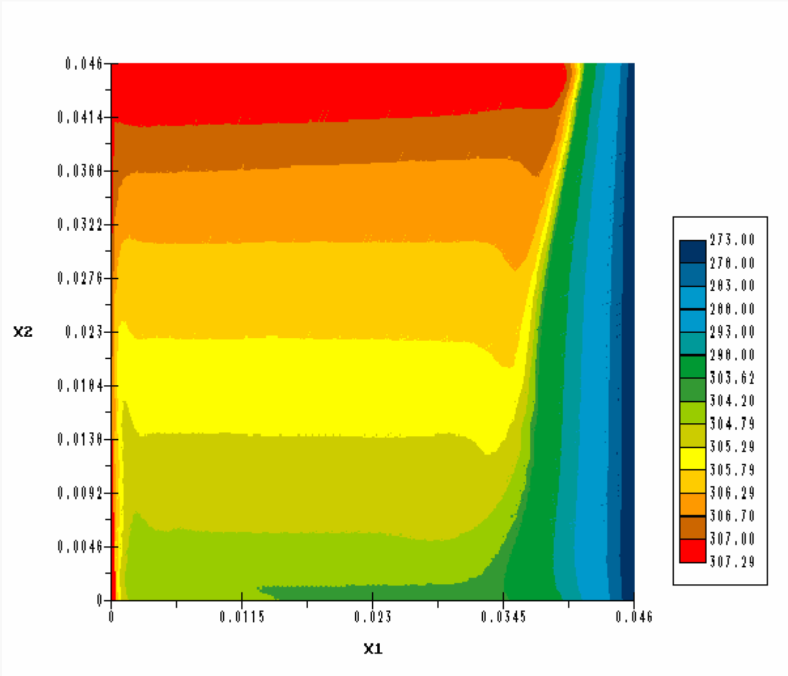
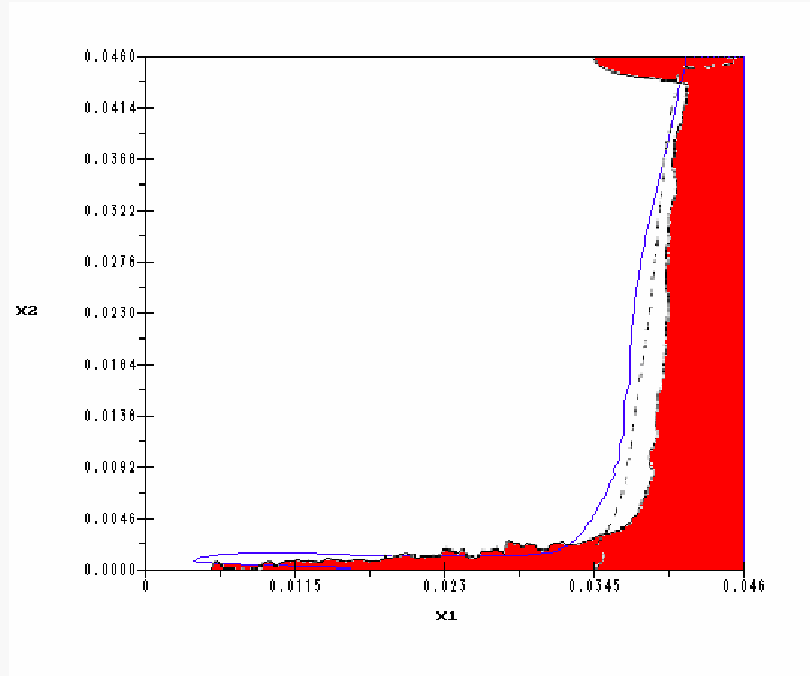




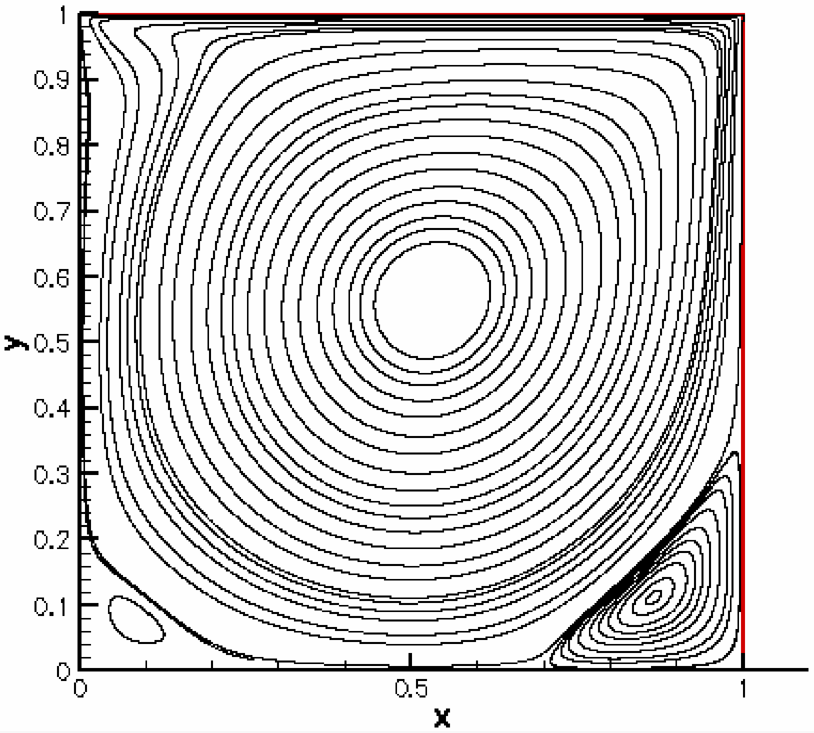
The numerical results obtained by means of CONVD code (blue line). Predictions for the total volume of mushy zone has a good agreement with Beckermann&Viskanta (*Physicochem. Hydrodyn., 10,195-213, 1988*) experiment (red field) and Lee&Tzong (*Int. J. Heat Mass Transfer*, *38(7), 1237-1247, 1995*) numerical predictions (dotted line).

DNS approach

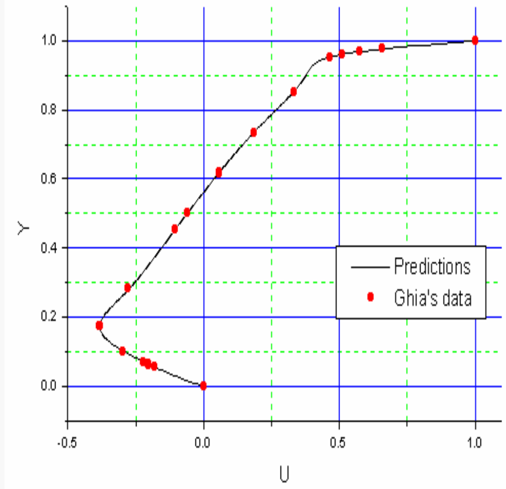
/2D Lid-driven cavity flow at Re=1000/

V.Ghia, et al., J.Comp.Phys., vol.48, 1982, 387-411

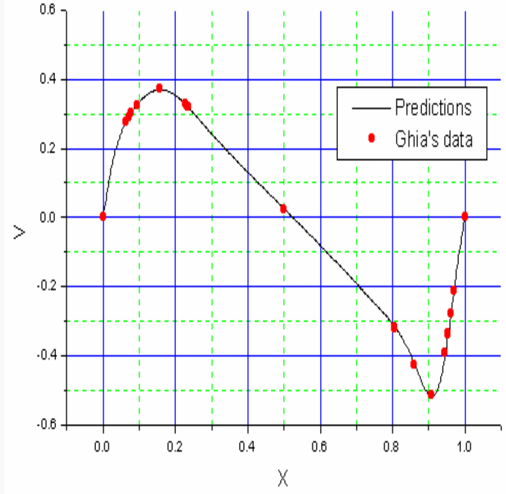
a)



b)



c)



a) Stream function;
b) U velocity along a vertical central line;
c) V velocity along a horizontal central line

3D Lid-driven cavity flow at Re=10000

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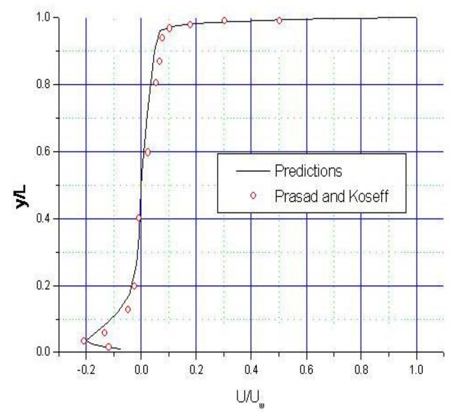
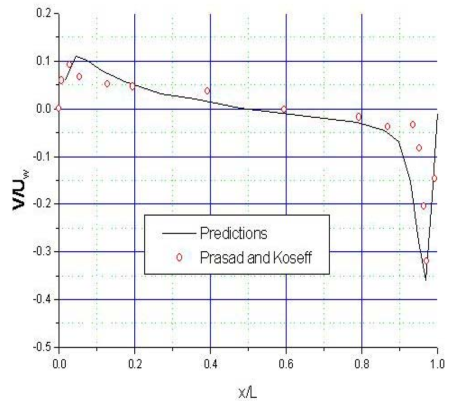
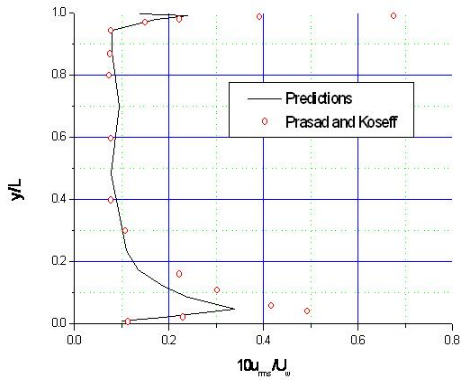
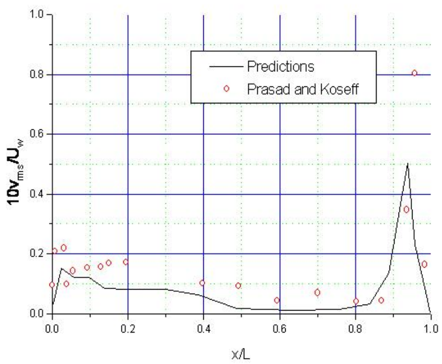
Prasad, A. and Koseff, J., 1989, J. Physics of Fluids A, Vol. 1, № 2, pp 208–218.









Top: U/U_w *-velocity along the vertical centerline.*
Bottom: V/U_w *-velocity along the horizontal centerline*

Top: $10u_{rms}/U_w$ *- along the vertical centerline.*
Bottom: $10v_{rms}/U_w$ *along the horizontal centerline*

3D Lid-driven cavity flow at Re=10000 (#2)

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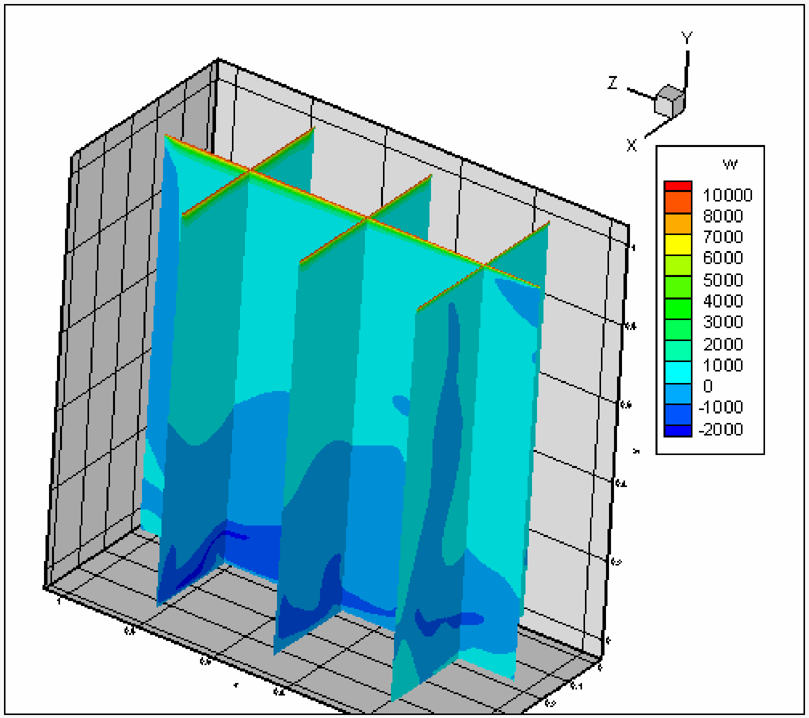
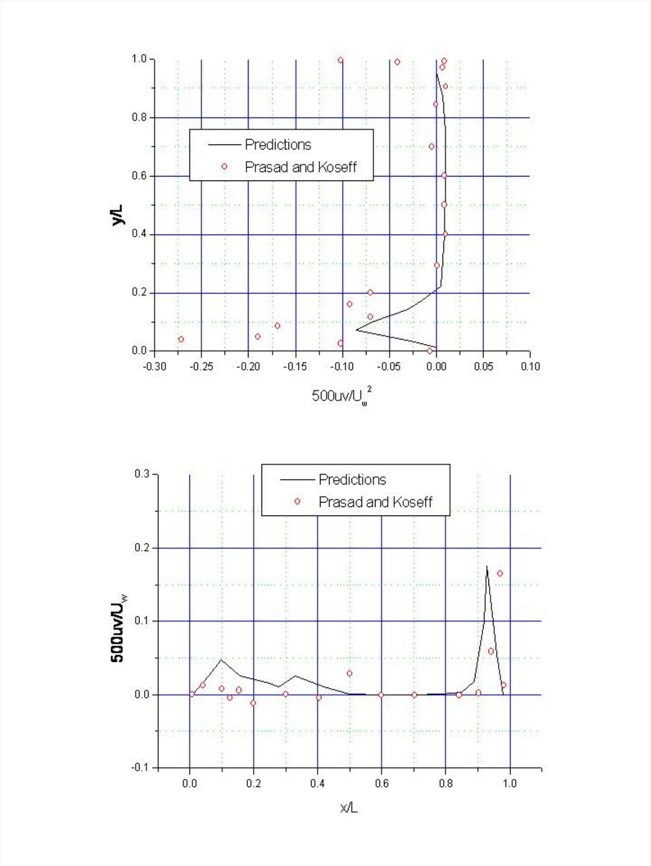


Three-dimensional field of W velocity component



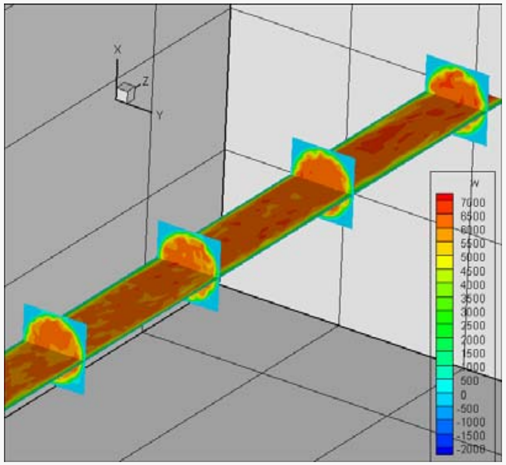
Top:500uv/U^2_w - along the vertical centerline.
Bottom:500uv/U^2_w along the horizontal centerline

Turbulent flow of water in a round pipe

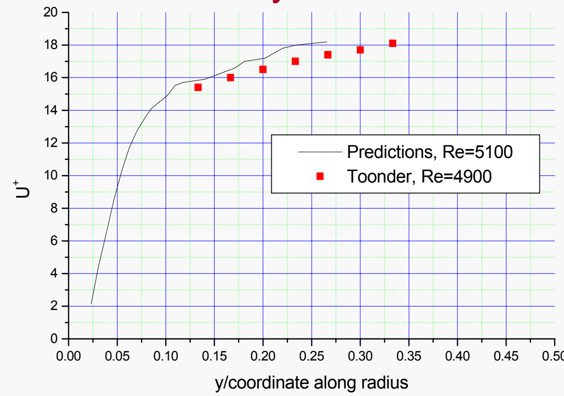
J.M.J. den Toonder et al., 1997, J. Phys. Fluids, 9(11), 3398-3409

Three-dimensional distribution of W velocity component in a round pipe at

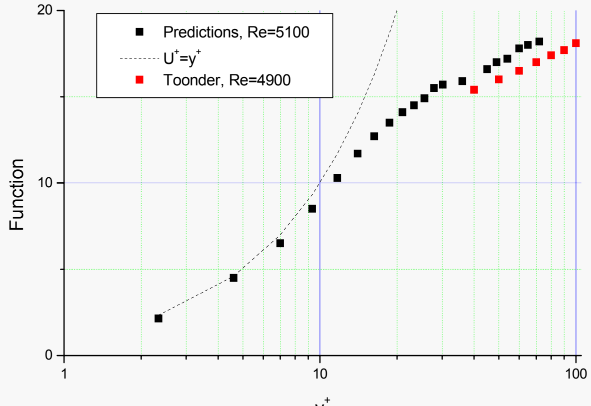
Re=5100



The distribution of a longitudinal component of a velocity on radius

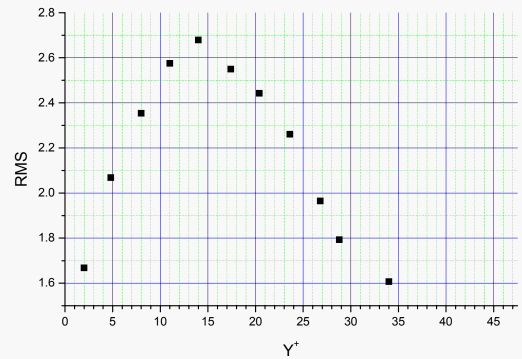


Mean-velocity profile, $U^+=f(y^+)$



$U+$ is the scaled mean velocity, $y+$ is the dimensionless distance to the wall, f is a universal function generally known as "the law of the wall"

Root-mean-square (rms) profile longitudinal component of a velocity



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LES approach

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$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \qquad (1)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \overline{\bar{u}_i \bar{u}_j}}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \bar{u}_i}{\partial x_j x_j} - c_\varepsilon \bar{u}_i \qquad (2)$$

where the effect of small scales appears through the SGS stress term given by

$$\bar{\tau}_{ij} = \overline{u_i u_j} - \overline{\bar{u}_i \bar{u}_j} \qquad (3)$$

In contrast standard LES, the nonlinear terms $\bar{u}_i \bar{u}_j$ and τ_{ij} are treated with a secondary filtering operation to eliminate the generation of frequencies higher than the characteristic wavenumber for the chosen filter.

The equations (1)-(3) govern the evolution of large scales of motion.

The boundary conditions for filtered velocity components can be taken to be the physical boundary conditions.

A Smagorinski model based on a eddy viscosity concept has been used as an SGS model.

Wall function may be used in a combination with LES approach, for example

$$f(y^+) = 1 - \exp(-y^+/25).$$

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Conclusions

IBRAE

- For modeling of phase change in binary alloys the numerical approach and computing module were developed, in which continuum model (Prakash&Voller, 1989) was used together with new developed in IBRAE numerical algorithm for modeling of multiphase flows. Numerical predictions were compared with experimental data (Beckermann&Viskana, 1988) and numerical data (Lee&Tzong, 1995). In both cases the good coincidence was observed.
- For simulation of turbulence flows was used as direct numerical simulation (DNS) approach and developed algebraic turbulence model. The applicability of the developed turbulence approach was proved by the extensive validation against the 2D and 3D results of lid-driven flows (Ghia, 1982) and flow in tube (Toonder, 1997).
- The possibility of modeling of the melt flows simultaneously with a heat transfer in the reactor vessel and crust formation at high Rayleigh numbers is realized in developed CONV code. The applicability of the realized approach was proved by the extensive validation against the results of molten-salt tests (Chudanov, 2000).