NUMERICAL BENCHMARK BASED ON NATURAL CONVECTION OF FREEZING WATER

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ABSTRACT
The proposed benchmark configuration concerns steady-state natural convection of water in the differentially heated cube-shaped cavity for temperatures close to the freezing point. Strongly non-linear buoyancy term allowed for thoughtful testing of several numerical approaches. After selecting the best performing one a new, very restrictive verification procedure is proposed. The verified numerical code is used to simulate the *"real world"* of an experimental configuration.

INTRODUCTION
The accurate solution of natural convection in enclosures is a crucial task in a goal of achieving precise modelling of solidification problems. Serious discrepancies between numerical and experimental results encountered for a *simple* problem of ice formation in a differentially heated cavity motivated us to revise reliability and performance of typical solvers used for simulating heat transfer phenomena. Traditionally such solvers are verified using reference solution defined by Graham de Vahl Davis [1] over 20 years ago. It appears that this largely simplified configuration does not permit to depict bad performing schemes, especially for strongly non-linear variation of the fluid density function. The aim of this work is to formulate a new benchmark solution for verification of numerical codes employed for modelling ice formation problems. The proposed benchmark configuration concerns steady-state natural convection of water in the differentially heated square cavity. By setting the temperature range of isothermal walls close to the freezing point and by adopting non-linear variation of the water density with temperature a challenging flow configuration with two counter-rotating re-circulation zones is obtained (comp. Fig. 1). The competing effects of positive and negative buoyancy force create interesting flow pattern with colliding hot and cold liquid jets. Several numerical codes were used to obtain accurate solution for this configuration. After selecting the best performing one a new, very restrictive verification procedure is proposed. It is based on calculating deviation of the velocity and temperature profiles extracted along three selected lines crossing computational domain. The profiles extracted for the accurate, *"benchmark"* solution are approximated with the high order polynomial and treated as a reference for an error evaluation. Results obtained for the competition of different numerical approaches as well as a reference to experimental data justify necessity for this type of profound code verification.

PROBLEM FORMULATION
We consider a steady-state, natural convection of water in the differentially heated cube-shaped cavity of a height L=38mm. Two vertical walls are isothermal, kept at temperatures $T_H = 10^oC$, $T_C = 0^oC$. Top and bottom walls are assumed to be adiabatic. In the physical experiment [2] the cavity is a Plexiglas cube and the isothermal walls are made of metal and kept at constant temperature by two thermostats. Air surrounding cavity and finite thermal conductivity of the Plexiglas walls modify thermal boundary conditions. This effect has been discussed in the previous papers by Kowalewski & Rebow [2], Leonardi et al.[3], Giangi et al.[4], Banaszek et al [5], and will be included in the numerical code after the code verification is performed.
Our prime aim is to verify performance of the numerical models and to estimate the accuracy of

the discrete approximate solutions in the presence of strong velocity and temperature gradients generated by the non-linear buoyancy term. The anomalous thermal variation of the water density is implemented in the buoyancy term using the fourth order polynomial given previously by Kowalewski & Rebow [2]. The verification of codes and benchmark definition is limited to simplified, two-dimensional case and idealised thermal boundary conditions, i.e. isothermal and adiabatic walls.

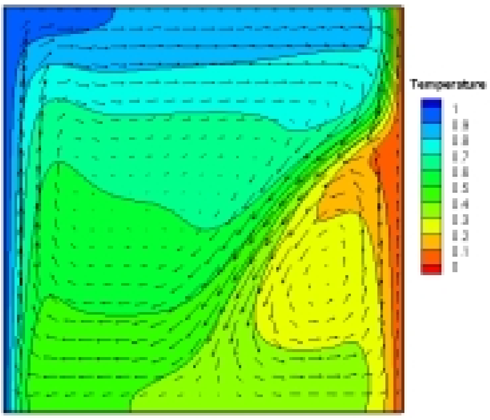

Figure 1
Natural convection of water. Temperature and velocity fields for the fine mesh solution of FRECON3V

Performance of five different numerical approaches was verified, using two commercial codes (Fluent [6] (FLU) and Fidap [6] (FID), the finite difference approximation code FRECON3V [3] (FRE), the finite difference, classical vorticity-streamfunction code SOLVSTR (STR), and the new mesh-free numerical approach (MEF) based on diffuse approximation method. The extensive mesh-sensitivity tests were performed for each of them and the result of the best performing algorithm was selected as a reference solution. Details will be presented in the forthcoming paper [7]. The selected reference code was FRECON3V, offering fast convergence to the "good" solution for 201x201 nodes mesh. This solution was selected as the benchmark and compared with other codes. It appeared that in order to compare performance of different codes in terms of their ability to reproduce fine details of the flow structure it is not sufficient to verify agreement of global flow field parameters, like those given in Tables 1.

Table 1
Global accuracy test by evaluating non-dimensional velocity extremes and Nusselt number for five investigated codes

Code	Nodes	U_{min}	U_{max}	W_{min}	W_{max}	Nu
FRE	21x21	-141.9	101.4	-225.6	215.2	7.05
FRE	41x41	-156.1	101.1	-177.0	213.1	6.98
FRE	**301x301**	**-159.2**	**103.4**	**-176.0**	**222.5**	**6.47**
FLU	38x38	-158.9	105.3	-172.4	208.1	6.59
FLU	380x380	-159.7	103.5	-174.7	223.5	6.50
FID	77x77	-159.0	105.4	-174.9	225.2	6.44
STR	250x250	-162.4	105.1	-177.4	227.6	6.65
MEF	100x100	-161.9	103.8	-167.6	225.9	6.22

Small deviations of global values from the reference solution, may correspond to distinct changes of the flow pattern. Such changes become responsible for differences in the local mass and heat transfer in the system. These effects can be perhaps neglected if only insulation or heat drainage are of the main interest. But they are not tolerable when phase change processes are present (e.g. freezing of water) or transport of small inclusions is an important issue. For example, if we compare Nusselt number of the most coarse solution FRE with that for a doubled mesh density (comp. Table 1), one may get impression that both solutions describe the same flow configuration. In fact these are two different flow fields. Location of the two circulation zones and the corresponding saddle point in the velocity fields are shifted, changing the whole flow pattern. Comparison of velocity profiles extracted for this sensitive region reveal up to 50% differences in the vertical velocity component. Hence, to obtain better insight into differences or similarities of the flow structures obtained from the investigated solvers, the second step of the verification procedure is proposed. It is based on calculating deviation of the velocity profiles extracted along three selected lines: horizontal centreline y=0.5, vertical centreline x=0.5 and vertical line passing through the mixing zone and the stagnation point at the cold wall (x=0.9). Locations of the lines are selected in such way that for any investigated mesh resolution they still match the nodes location, and additional interpolation errors are avoided. The velocity and temperature profiles extracted along above mentioned lines are approximated with the high order polynomial and treated as a reference (benchmark) solution. The numerical values of the polynomials coefficients are available for quick and accurate evaluation of errors.

An assessment on the accuracy of the solution is obtained calculating relative differences in terms of standard deviations, evaluated for the polynomials describing benchmark profiles and corresponding values extracted from the interrogated solution.

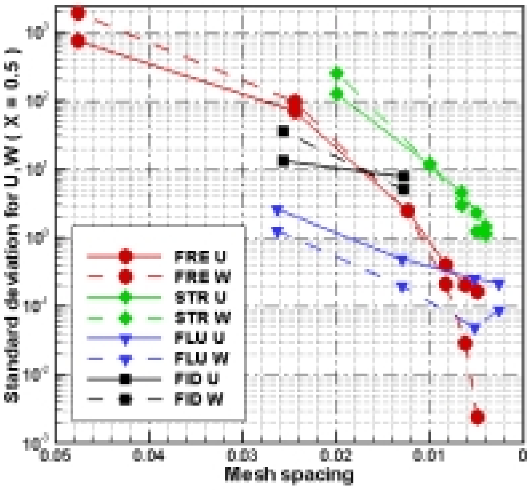

Figure 2
Error estimation for velocity profiles along vertical, centre line evaluated for the four analysed codes.

Figures 2 easily indicates differences in convergence rates between four codes, however each of them claims second-order approximations. It is worth noting that convergence of temperature is relatively easy to reach, and even for the most coarse meshes temperature profiles are practically "exact". It indicates robustness of the energy equations and relatively small effect of the convective term on the resulting temperature distribution. It is rather surprising result, and it suggest that use of temperature as a convergence indicator can be dangerously misleading. At least for the analysed flow configuration. Four analysed codes finally reached solutions close to our benchmark, but only two (FRECON3V and Fluent) qualified as *"good"*, if we apply stricter cut off criterion (three standard deviations). The mesh-free code MEF completely failed our tests of accuracy. On the other hand, its extremely long calculations time does not allowed for further mesh refinements.

EXPERIMENTAL VALIDATION

Numerical solution, even very strictly verified, has only an academic value as long as it is not validated, i.e. confronted with the *"real world"* physics. Before we can answer the prime question of the validation procedure, *"is our code solving a proper set of equations"*, careful analysis of all physical details of analysed phenomena must be performed. To make it clear, it is not possible to match physical phenomena to an idealized numerical benchmark. Nothing like isothermal or adiabatic wall exists in reality, fluids are not ideal and their variable properties must be known. Hence, the question arises, how exact description of the physical phenomena is necessary. The answer may be drawn from numerical sensitivity tests only. Due to the non-linearties of governing equations estimation of errors produced by model simplifications is difficult, sometimes very disappointing.

Hence, before applying numerical model to simulate physical experiment a careful sensitivity analysis of numerical results was performed to determine the most important parameters describing our configuration. Moreover, we estimate the precision required for description of those parameters to conduct a full validation procedure. Additionally, our sensitivity analysis allowed to choose the most suitable configuration for comparative studies, to say configuration which is the least sensitive for changes in experimental conditions what significantly simplify and help in our laboratory investigations. Sensitivity analysis was conducted for the sake of boundary condition, initial condition and fluid properties. Based on our previous experience [2-5] we took into account in our computational model not only fluid domain described in previous section but also isothermal and adiabatic walls. Figure 3 shows altered configuration with two isothermal walls and two adiabatic walls, which was suitable for thorough comparisons. The sensitivity analysis revealed that such system strongly depends on thermal boundary condition imposed on external walls. Heat fluxes not only through *"adiabatic"* but also trough *"isothermal"* walls have to be analysed. It appeared that small variations in heat fluxes Q_1, Q_2, Q_3 (less than 100 W/m^2) considerably changed the flow structure inside the fluid square domain. The flow structure consisting of two counter-rotating circulations, described in previous section, turned out to be very sensitive and underwent changes even only due to small variation in one of these heat fluxes. Hence, the first requirement for laboratory experiments is a precise knowledge of heat fluxes to/from the enclosure, including internal construction of metal blocks responsible for thermal stabilization of *"isothermal"* walls. The requested precision in heat flux measurements was estimated and correct heat transfer coefficients measured in separate experiments for both, so called, "*adiabatic*" and "*isothermal*" walls. Sensitivity analysis for the sake of material properties was conducted by comparing results with assumed constant values of viscosity, specific heat and thermal conductivity with that with variable fluid properties. Variability of specific heat and thermal conductivity did not altered flow structure significantly whereas variability of viscosity caused 8% decrease in velocity magnitude and has to be considered in the numerical model.

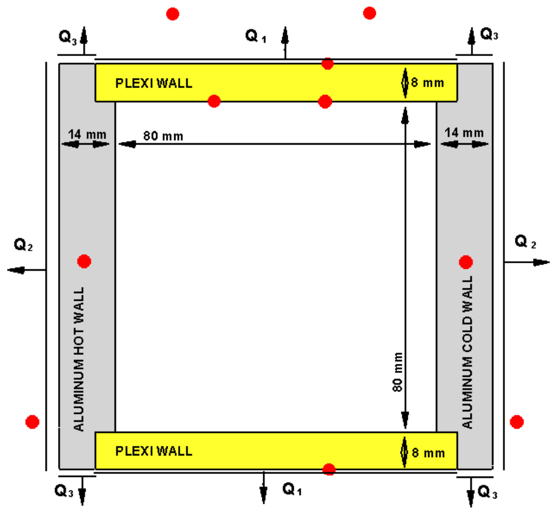

Figure 3
Sketch of physical geometry used in the validation experiment

Initial condition appeared to have minor influence to final results of our calculations. Even strong perturbation imposed in the initial temperature field did not cause any noticeable alterations in final steady states.

Taking into account results of the sensitivity analysis of the numerical model the experimental setup was designed in order to meet all mentioned requirements of full validation process. Experimental setup consist of cubic cavity with internal size 0.08 x 0.08 x 0.08 m, with two opposite side-walls made of a 14 mm thick aluminium, and four remaining walls made of a 8 mm thick Plexiglas. The left side aluminium wall was heated by coolant kept on the constant temperature T_H = 10°C, whereas the right side aluminium wall was cooled by coolant kept on the constant temperature T_C = -2°C. A set of thermocouples was installed in the aluminium walls, the Plexiglas walls, and in the vicinity of the cavity in order to monitor local air temperature and precisely calculate heat fluxes. Position of thermocouples in central cross-section of the cavity was depicted in Figure 3 (red circles). Steady state convection was assumed after running the experiment for several hours. The Rayleigh and Prandtl numbers calculated for the experimental parameters are $1.2\text{x}10^7$ and 13.32, respectively. The Rayleigh number is based on the obtained temperature difference between the internal aluminium walls ΔT = 10°C and fluid properties at the reference temperature T_0 = 0°C.

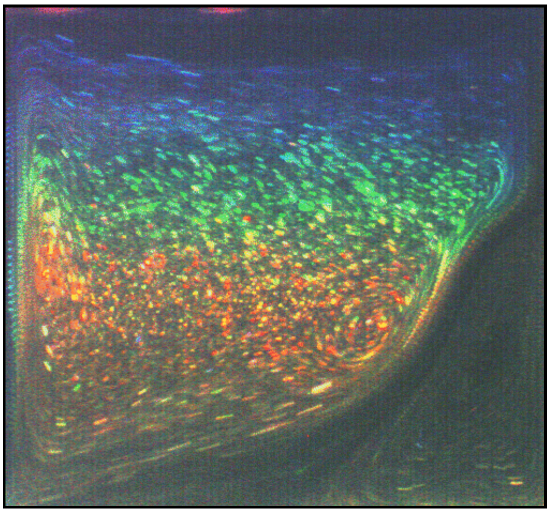

Figure 4
Digital image of flow field seeded with liquid crystal tracers

Thermochromic liquid crystals were used as tracers in order to measure simultaneously two-dimensional velocity and temperature fields. Quantitative experimental data on velocity and temperature fields in a central cross-section was obtained by making use of Particle Image Velocimetry (PIV) and Particle Image Thermometry (PIT) techniques [8]. Figures 4 presents an experimental image of liquid crystal tracers changing their colour with temperature between 4°C and 9°C (red 4°C-6.0°C, yellow 6.0°C – 6.5°C, green 6.5°C–7.5°C, blue 7.5°C-9°C). Pair of such images was used to obtained velocity field by PIV technique. Resulting 2D velocity field is showed in Fig. 5. Additionally, temperature was monitored during whole experiment in points depicted in Fig. 3 (red circles) by set of thermocouples. That allowed to estimate heat transfer coefficients α_1 = 10 W/m^{2}K, α_2 = 2500 W/m^{2}K, α_3 = 1400 W/m^{2}K necessary to calculate respectively heat fluxes Q_1, Q_2, Q_3 with required accuracy.

Accurate experimental measurements allowed for application of appropriate boundary conditions into the previously verified computational model. Fluent was chosen for its flexibility in modelling geometry of the cavity. Numerical simulation resulted in quantitative agreement between experiment and numerical simulation, impossible to achieve by *ad hoc* estimations made in a first attempt. Example of computed velocity and temperature fields is given in Figure 6.

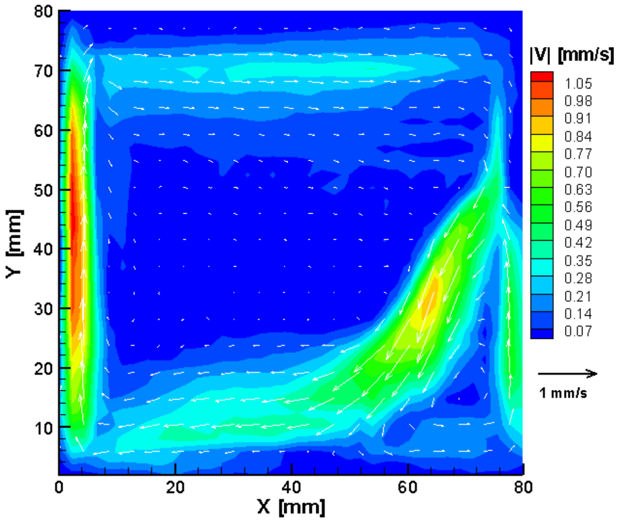

Figure 5

Velocity field measured (PIV) in the centre cross section and velocity magnitude contours

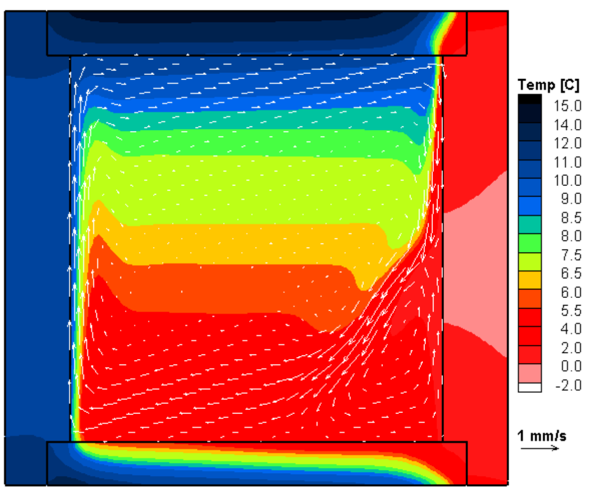

Figure 6

Velocity and temperature fields computed for *physical* configuration, used for the code validation procedure

CONLUSIONS

New numerical benchmark based on natural convection of water in the vicinity of freezing point is presented for verification of numerical codes. The sensitivity analysis was used to choose the most appropriate experimental configuration for validation of performed calculations and to determine necessary precision of measurements. Quantitative agreement between experimental and computed results allowed to validate described calculations.

ACKNOWLEDGMENTS

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