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Validation problems in computational fluid mechanics

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Recent developments in Computational Fluid Dynamics (CFD) increased interest in quantifying quality of the numerical models. One of the necessary steps is the so-called *code validation* procedure, an assessment of a numerical simulation by comparisons between simulation results and laboratory measurements. The focus of the present review is application of modern full field experimental techniques, mostly based on the digital image analysis, in validating numerical solutions of complex flow configurations. Each validation procedure opens new issues of quantifying its outcome to find directions for model updating, limits of computer simulation quality, and to perform uncertainty quantification.

Keywords: CFD validation, experimental methods.

1. INTRODUCTION

In many fields of computational sciences, numerical models are developed for predicting the response of a system when the phenomenon is not accessible by direct measurement or when numerical simulations are less expensive than testing. With the growing capacity of computers and continuing improvement in numerical codes, the question of the accuracy of numerical solutions is of primary importance.

The usefulness of the numerical solution depends on its ability to model physical problem. The number of commercial codes is available for solving almost every problem imaginable in the field and may suggest that the époque of expensive and complicated laboratory experimentation has passed. Although we all would welcome such a development, the credibility of the numerical results remains a concern tempering some of this optimism. Typical difficulties in obtaining credible predictions for industrial problems lead to the often encountered dilemma: Do we trust numerical simulations? Of course, this is not specific for fluid mechanics only. However, strong nonlinearities of governing fluid flow equations, inevitable model simplifications necessary to solve turbulent flow, presence of complex couplings of mechanical interactions with thermal, surface, chemical, gravitational or multibody effects create multiple sources of uncertainties and serious errors. Problem of uncertainties is often neglected if applicability of the simulation results following from more or less idealised models is limited only to the global description of the investigated problem.

Developing sophisticated numerical models does not necessarily guarantee accuracy and predictability. It must somehow be verified that the many assumptions involved in the successive steps of idealisation, discretisation, and modelling yield satisfactory predictions. This is known as model verification and it is usually carried out by comparing the predictions of a model or family of models to reference data. If the agreement between the two sets is not satisfactory, design parameters can be optimised to improve the predictive quality of the models.

Still any verification result will not improve physics of the model! The human tendency is to justify solution as correct just because it has converged and produced high-quality colour plots. Limitations of the specific numerical model are not easily considered, hence frequently only very general description of the flow is judged. However, nearly the same pressure drop, heat flux or drag force can be found for the completely different flow structure. There is a wide class of practical problems where knowledge of just the general behaviour of flow is not sufficient to obtain a full quantitative explanation of the phenomena. Examples include the distribution of fuel or soot in a combustion chamber, the transport of impurities in crystal growth, the propagation of pollution in fluid flow, or effects of small scale flow phenomena on the bulk flow. The knowledge of some specific flow details appears to be necessary for the full control of the investigated phenomenon. Improvement in the accuracy of theoretical and numerical models and their experimental validation is an indispensable procedure in such cases. This issue seems to be especially pertinent when modelling multiphase and multi-scale phenomena.

2. Verification & validation

During the past two decades there has been a growing interest in verification and validation (V&V) as a distinct part of computational fluid mechanics. The evidence for this increased interest is the formulation of several initiatives to establish methods of code verification (i.e., checking method and accuracy of solvers). Since the beginning of the computational fluid dynamics verification of the code was an important issue. Several, the so-called "numerical benchmarks" appeared, the first and probably best known was given by Graham de Vahl Davis [1]. Having reference solution based on apparently accurate code (usually obtained using high resolution discretisation) other code developers could evaluate performance and accuracy of their products. The aim of the code verification seems obvious; each numerical analysis using the same physical model should produce consistent result. Nowadays a plethora of numerical benchmarks are available covering most of the typical cases. One of them worth to mention is collection of cases given by ERCOFTAC [2].

Generally speaking code verification should establish confidence that the mathematical model and the algorithms responsible for discrete solution are working correctly. Neither part of verification process addresses the question of the adequacy of the selected conceptual and mathematical models for representing the reality of interest. This part of the code evaluation touches the second component of the V&V abbreviation, namely code validation. The term code validation, defined probably for the first time in the early 1980s by Boehm [3], is understood as determining the degree to which the analysed numerical model is an accurate representation of the real world. For a long time both terms- verification and validation, were mixed in the computer science literature without deeper understanding of differences between them. As it was underlined by Roache [4] we have to confirm that not only equations are solved correctly but, what is even more important for practice, that we are solving the right equations. Hence, there is an essential distinction which can perhaps, in the simplest way given, define scope of the methods used: the code verification is based on a mathematical analysis; the code validation is based on experimental outcomes.

The both V&V procedures are necessary to perform Code Qualification, the last step before applying it to solve real engineering problem. This last step is the main goal of engineering applications, as it has to compare physical model used for the validation with the real industrial configuration. Finding proper methodology to perform this practical issue is problem specific, sometimes very difficult to realise. Here, we concentrate on the code validation issues, trying to elucidate problems with preparing proper experimental reference allowing to "validate" physics of the model. Performing code validation we may define three distinct issues.

The first obvious one is to construct model experiment including all expected physical ingredients of the analysed phenomena. We still use a term "model", as in the most cases it is very difficult or sometimes impossible to operate with the final target of the simulations. Usually size, extreme values of parameters (temperature, gravity), accessibility of the interrogated flow region, and so on, force us to mimic physical phenomena at a laboratory scale. It allows for better control of all physical conditions and to apply data acquisition methods not applicable in industrial, geophysical or space environment. The second issue of the code validation, namely the accuracy assessment, is not less important. Having experimental and numerical data we have to define a proper methodology to find the validation metric in terms of the data accuracy and sensitivity of the analysed model outcome to inevitable experimental errors. This part of the assessment is coupled with the first one, as it defines limits of the experimental accuracy necessary to perform validation procedure. Finally, we have to define procedure for the further analysis. Practical limits of agreement/disagreement between model and reality have to be verified. If the sensitivity analysis suggests improvement of accuracy of specific experimental data, the validation experiment should be redesigned. However, it is possible that the model does not cover all the necessary details of the physical environment. Then, it is necessary to extend both the mathematical description of the analysed phenomena as well as the experimental methodology of monitoring effects related to the new ingredients. From this point the validation loop starts from the beginning. The number of repetitions is unknown, convergence of the procedure cannot be granted too. In some cases discrepancy may even explode, indicating that previous agreement obtained for a less complex model in fact hindered proper description of the physical phenomenon. Hence, identification of parameters playing crucial role in the specific flow problem is necessary.

It is necessary to perform sensitivity analysis of the problem, delivering information about tolerance span for the accuracy in description of boundary conditions, flow geometry, and material properties. Without sensitivity analysis it is difficult or impossible to define experimental benchmark which delivers data sufficiently accurate for the proper code validation. On the other hand sensitivity analysis in fluid mechanics can be performed only using high-resolution *exact* solutions obtained using *Direct Numerical Simulation* (DNS) solvers. These relatively new numerical methods may sometimes even replace experiment. Performing reference DNS simulations, despite of huge demand of computational resources, is often essential for determining code validation experimental procedure for turbulent flows.

Let us illustrate what is said above on a simple imaginary example. We would like to validate solution obtained numerically for a steady flow of viscous fluid through a straight cylinder of the circular cross-section. In simple words, it is a pipe flow described for an infinite cylinder by uni-component parabolic velocity profile. For brevity of the description let us assume we already have numerical solution obtained for example by finite volume method using unstructured mesh. The method is expected to have limited accuracy due to the singularity at the tube axis, hence first of all the code verification has to be performed. To conclude the problem we have to define inlet and outlet boundary conditions, let us say constant velocity (plug flow) at the inlet and equivalent volumetric outflow at the outlet. Finally, the pressure drop and velocity profile within the whole tube have to be extracted from the numerical solution and compared with the experimental data. Development of the flow velocity profile at the entry is already quite complex and validation of the numerical prediction may appear to be a nightmare. Hence, let us compare only global values. We take calculated and measured pressure drop between two locations defined on the tube surface. Probably error would be negligibly small if our experimental device could measure pressure without disturbing the flow. In practice any hole or connector attached to the tube disturbs the flow. Is such disturbance important? To answer such a trivial question we have to perform new numerical simulation modifying the wall geometry. To make it more complicated (and accurate) we should also ask CFD modeller to include wall deformation due to the compliance of the sensor area in any pressure gauge. To evaluate effects of these two new factors included in the numerical model it is necessary to perform sensitivity analysis. It partly could answer the second question: is our experimental methodology accurate enough to validate the improved flow model? Probably not, hence either we agree that our code is accurate enough to predict the pressure drop with error bars found by the sensitivity analysis. Or we look for more sensitive parameter like fluid velocity close to the obstacle created by the pressure sensor.

Proper selection of the experimental data is crucial in any sensitivity analysis. Comparing few single point data (e.g., velocity at selected flow points), quite often used in the past, is misleading. It is suggested that at least two- or three-dimensional profile of data is extracted along well selected (i.e., sensitive to flow conditions) cross section of the flow. Sampling of the experimental data should be in agreement with the numerical resolution of the validated code. Comparing standard deviations for the whole profiles between numerical and experimental data allows to quantify degree of agreement and to evaluate improvement of results generated with different physical models. Finally, we have to define proper validation metrics allowing for rigorous sensitivity analysis. Solving the flow problem for various values of selected parameters of the physical model we are able to create multidimensional map describing sensitivity of the solution to the variation of selected modelling parameters.

Generally, any flow perturbations not included in the general description of the phenomenon may appear due to non-ideal boundary conditions, initial conditions, and variations of physical properties of wall or fluid. Moreover, we may expect additional flow perturbation mechanisms like gravitational, electro-osmotic, thermal, rotational (Coriolis force) etc. Hence, after several iterations trying to improve physics of our numerical model we may come to the conclusion that the accuracy of our numerical solution has obvious limitations. It remains to be decided if errors produced by the model limitations are acceptable for our practical application or the numerical method must be confronted with *ad hoc* implemented "scaling factors", silently covering our lack of competence.

We hope that this simple example helps to convince CFD modellers to analyse sensitivity of the solutions not only to inevitable errors due to numerical approximations, but also due to inevitable simplifications of the physical model used to describe the "real world". It implies construction of experimental models including most of the physical details relevant to the "real world" problem under consideration. Some classes of the experimental models with detailed description of the interacting forces, flow structure, and material properties form the so-called "experimental benchmarks", reference experiments for the validation procedure. Unfortunately, there is no universal validation procedure. Each analysed case needs an individual approach. However, we may try to identify some classes of phenomena where similar validation procedure may become applicable. The most common and straightforward class describes both bounded and unbounded flows, where some characteristic driving mechanism generates fluid motion. Usually it involves flow in ducts, closed containers, flow along single wall, with driving force given by pressure difference or mass force like gravity, magnetic or electrostatic forces. The flow geometry is fixed and we deal with uncertainties due to the simplifications of the physical description. The parameters we have to monitor involve local velocity field and other fields depending on the external forcing, e.g., pressure, temperature, concentration, magnetic, electric and other specifics for problem fields. Other class of flows which needs specific care to create a validating experiment involves flow-structure interactions. Besides details about flow field it becomes necessary to obtain accurate description of mechanical properties of the structure and its dynamically varying geometry. Free surface flows (bubbles, drops, liquid jets) create subclass of the above. Flow field interacts with the bounding it surface and the surface forces are driving the flow. Details on surface properties, geometry, dynamic changes become crucial for the validating experiment. Hence, it is necessary to develop experimental procedure allowing for appropriate analysis of surface deformation.

In the following, a few cases are given to exemplify methodology we used to construct experimental benchmarks. First, we look at free surface flow showing possibility to construct well defined surface parameterization, compatible with the numerical description. Few other validation examples describe thermally driven flows. Finally, we show an example of the sensitivity analysis performed for a simple, convective flow.

3. Towards experimental benchmarks

With recent progress of experimental methods introduced by digital image recording and analysis techniques, validation of numerical codes using full field experimental data became one of the most challenging research goals. In a few examples we aim to demonstrate methodology and outcome of validation procedure based on image analysis.

3.1. Free surface flow

Perhaps most straightforward demonstration of the proper selection of the validation metrics offers problem of modelling oscillation of a liquid droplet (cf. Fig. 1). Single droplet suspended in air can be treated as an insulated mechanical oscillator driven by surface forces and kinetic energy of the internal flow. Every such an analysis has to start from the statements of mass and momentum conservation in form of the equation of continuity and the Navier-Stokes equation. The Navier-Stokes equation is scaled using droplet radius, velocity with maximum deformation amplitude, and pressure depending on surface tension and local curvature of droplet surface. Limiting our considerations to axisymmetric deformations, droplet surface deformations can be described as an infinite series of the surface spherical harmonics [5]. Motion of the droplet surface and flow velocity are coupled by the kinematic boundary condition, evaluated for each time step for new surface deformation. Due to nonlinearities arising from inertia, capillarity and coupling of the surface kinematics to the velocity field, solution of the problem equations is a non-trivial free-boundary problem. Only by assuming small amplitudes of droplet deformation and neglecting viscous damping, the problem becomes linear and can be solved analytically. The widely known linear, irrotational approximation given by Lamb [5] describes the instantaneous deformation of the droplet shape by an infinite series of the surface spherical harmonics. Each term of the series describes one mode of droplet oscillation, characterized by its amplitude. Hence, the oscillation frequency of each mode and the decay time are simply defined as a sum of amplitudes for all considered oscillation modes. Higher oscillations modes are strongly damped. Therefore, in practice description of the "natural" droplet oscillation can be limited to the first few modes. Such a brief description is allowed for complete description of the droplet dynamics by extracting from the experiment only variation in time of the oscillation amplitude of each mode [6]. For the validation purpose crucial becomes selection of a proper sampling time and accuracy of the shape fitting to the multimodal deformation function given by the surface harmonics.

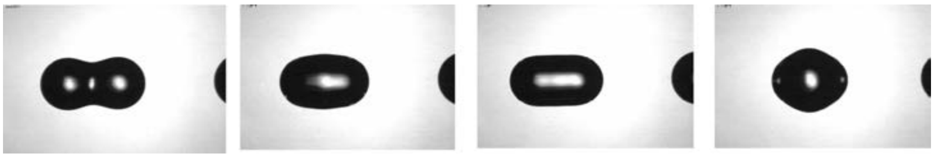


Fig. 1. Water droplet of 0.2 mm diameter oscillating in air. All observed deformation forms can be parameterised using single amplitude for each oscillation mode.

Even simple, linear models of oscillating droplet recognise complexity of this fluidic oscillator [5]. In fact surface deformation can be described by an infinite series of surface spherical harmonics, each of them uniquely described by their amplitude and damping. Limits of applicability of the numerical models are usually difficult to estimate *a priori*. Hence, beside the model development efforts, their validation is not the least problem. In case of droplet oscillations, nonlinearity of equation of motion cannot be simply described by a single parameter, i.e., Reynolds number. At finite oscillation amplitude both, the relative value of nonlinear terms of the Navier-Stokes equation and coupling through the boundary conditions, dominate droplet dynamics. Therefore, usual estimates of "strong" or "weak" nonlinear effects are misleading. For example, nonlinearity of higher oscillation modes remains even at infinitesimal amplitudes. Experiments with oscillating droplets show sequence of images of deformed droplets (Fig. 1). Comparing such images with numerical plots of the droplet surface does not offer quantitative measure of the model quality. To obtain reliable validating data from the experiment it became necessary to use the same metrics as used in the models. It is possible if the observed droplet shape is given in terms of spherical harmonics and only the parameters of the harmonics are used for validation purposes (Fig. 2). Hence, applying such approach it was possible to consider applicability of three theoretical models, namely M1 – a full model solving nonlinear N-S equation [6], M2 – simplified irrotational nonlinear approximation described in [7], and M3 – classical linear model of Lamb [5]. Applying mode description for

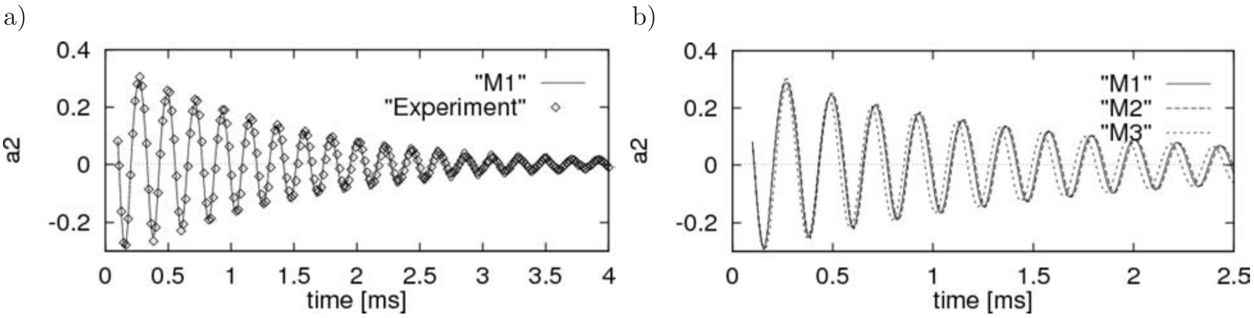


Fig. 2. Amplitude of oscillations evaluated from the experiment for the second mode a_2. a) validating nonlinear model M1 using the same shape parameterization; b) verifying simplified models M2 and M3 with help of validated benchmark solution [7].

experimental data it was possible to validate results of the model M1. Both large amplitude low modes as well as strongly damped higher modes are reproduced with accuracy easy to estimate by comparing appropriate curves. It gave us confidence that main parts of the physical model are included in the numerical model M1. Then, applying M1 as numerically trusted model (numerical benchmark), we can also verify limits of the irrotational approximations. It is worth to mention that selected validation procedure is sensitive enough to look deeper at the analysed phenomenon and extend physical description beyond the Navier-Stokes equation. It was observed that oscillation of droplets consisting of liquid mixtures diffusive effects have to be included to describe time dependent adsorption of surface active substances [8]. Other phenomena not included are associated with evaporation and cooling effects. Heat and mass transfer change dynamics of the oscillations and influence physical properties of the liquid. In practice, these effects if properly modelled can be applied to develop experimental methods for determining dynamic surface tension [8], and to measure surface temperature of evaporating droplets. Both parameters are inaccessible by classical means. On other hand validated numerical model offers relatively simple tool to perform the sensitivity analysis and estimate accuracy of measurements.

3.2. Thermally driven flow

Modelling of thermally driven flows is of great importance for several practical applications, including construction of efficient heat exchangers, thermal insulation, or moderating chemical reactions. Proper modelling of thermally driven fluid flows coupled with phase change phenomena plays a crucial role in numerical simulations describing formation of semiconductor crystals, casting processes, or environmental effects of ice formation. For over two decades various computer simulations of these coupled and complex phenomena have become a fundamental tool for prediction of local flow patterns, temperature and concentration fields, supplementing or even replacing cumbersome, time-consuming and expensive experimental findings. However, accuracy of predictions is still an issue. And the main problem is not due to the inefficient algorithms but due to inaccurate physical models being solved. Hence, validation of numerical models developed for these applications is of great importance.

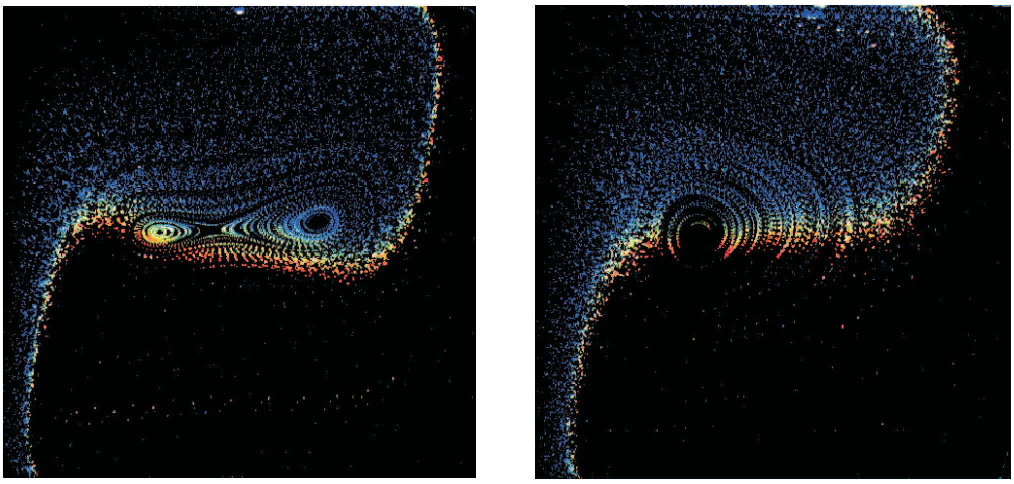
Simultaneous measurement of the flow and temperature fields enables a relatively accurate verification of global features of experimental and numerical simulations for thermally driven flow. However, as we show even simple configurations may generate challenging problems for code validation. As an example let us consider the popular numerical “benchmark” case [1], stationary low Rayleigh number natural convection in a cubical cavity with differentially heated side walls. Two opposite vertical walls are isothermal and kept at temperatures T_h and T_c, the other four walls are nominally insulators of finite thermal diffusivity. A heat flux, both through and along the walls, is generated due to temperature gradients existing between the fluid inside the cavity and the surrounding environment and also along the front and back walls, the lid and the floor of the box. The simple question arises if the numerical model with widely used adiabatic approximation of thermal boundary conditions for "nominal insulators" offers physically valid results [9–11].

Our numerical simulation of the problem was performed using a three-dimensional finite difference vorticity-vector potential formulation of the Navier-Stokes and energy equations for laminar flow of a viscous, incompressible fluid. The applied false-transient code was verified as superior in terms of accuracy and speed when applied to steady laminar flow [12]. To check the validity of the numerical solution in comparison with the experimental results, several methods of numerical visualisation were applied. In the first step the general flow characteristics, such as the two-dimensional temperature and velocity fields, were extracted. A detailed visualisation of the calculated flow structures was achieved using particle tracks obtained through the integration of the velocity equations. Despite simplicity of the problem serious discrepancies between measured and calculated flow structures became evident. After verifying several issues of the computational code as variable fluid properties, channel fabrication inaccuracy, temperature stability we came to the conclusion that possible effect may appear due to the finite heat fluxes within insulating side walls. Hence, the validation procedure is concentrated on the issue of the proper definition of thermal boundary conditions (TBC). The effect of proper modelling of the TBCs was analysed comparing measured and calculated flow patterns and velocity profiles. It came out that only slight modification of the heat fluxes through the passive walls considerably alters three-dimensional flow structure resulting large variation of the generated particle tracks.

The first, usually accepted, approach was to change simplified numerical model with adiabatic walls to the model using estimated heat losses through these walls. Such a one-dimensional heat transfer approach still could not properly reproduce experimentally observed flow tracks. It is necessary to underline that modification of the passive TBC influence flow structure only. The core flow transporting heat from hot to cold wall remains well predictable for any given imposed heat flux in the "insulating walls", and generally can be well approximated using simple two-dimensional modelling of the symmetry plane. Also evaluated global flow characteristics like velocity extremes, global heat flux (Nusselt number) vary only within 5% error for different models of TBC. However, looking closer at three-dimensional flow structure serious discrepancies between experiment and modelling were present.

The simplifications introduced by modelling TBCs at the side walls are responsible for variation of the three-dimensional flow structure. It consists of one or two spiralling motions which change its shape and pitch depending on the modelling of residual heat fluxes on insulated walls. At lower Rayleigh numbers ($\mathrm{Ra} = 21{,}000$), a computed single straight spiral transporting liquid across cavity has a different pitch compared with experiments [9], and its ends are curved. At $\mathrm{Ra} = 80{,}000$, the computed solution shows two rolls (Fig. 4a) whereas in the experiment, only one spiral initially appears at the front and back walls (cf. Fig. 3b). The spiral detaching from the wall splits midway along its length into two spirals forming characteristic "cats eyes" in the symmetry plane. Several numerical investigations elucidated that the cross-flow component of the flow velocity which is mainly responsible for the three-dimensional behaviour of the tracks is extremely sensitive to TBCs on all passive walls (cf. Fig. 4). Numerical experiments indicated that depending on the value and direction of the wall heat flux, the location of the core of the spirals at the side walls may be shifted towards the hot or cold side. In this way their pitch and even cross flow direction may be easily changed. Due to this sensitivity the estimation of the proper TBCs for the given experiment becomes a non-trivial task, especially for higher Rayleigh number.

To verify that the observed discrepancies are mainly due to inaccurate modelling of TBC, numerical simulation was performed with the temperature distribution set at all four non-isothermal walls as explicitly measured. It appeared that both the direction of the calculated spirals and their pitch correlate well with the measured particle tracks [10]. The improvement obtained gave us an indication of the necessity of introducing modifications to the modelling of heat transport through and along non-isothermal walls. In fact full 3D modelling of heat conduction through the insulating side walls provided numerical result not only valid in terms of global parameters (heat fluxes, velocity extremes), but also allowing to predict accurately motion of fluid particles [11]. This becomes espe-


a) centre cross-section

b) close to the front wall

Fig. 3. Flow structure visualised with thermochromic tracers for the convective flow in the differentially heated cubic cavity; (a) the centre plane cross-section and (b) the front wall; effect of thermal boundary conditions at side-walls, apparently double spiralling structure visible for the central plane merges to single roll close to the side wall [9]. The tracers colour indicates temperature.

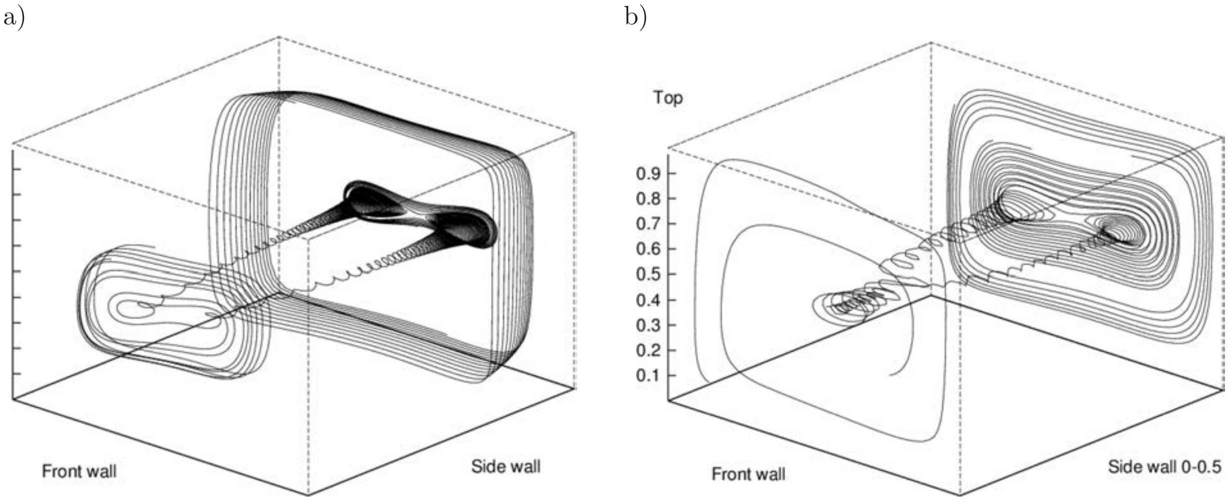


Fig. 4. Numerical tracks obtained for simulation of flow in the differentially heated cavity: a) assuming adiabatic TBC for Plexiglas side walls, and b) heat losses though the side walls. One half of the cavity is shown, merging of cross-flow spirals visible for non-adiabatic side walls.

cially important for several practical issues like transport of suspensions, collection of impurities, or purity of crystals grown in the convective flow. Slight changes of the components concentration may completely overwhelm quality of the semiconductors or alloys. Hence, proper validation of numerical codes applied for modelling flow problems with phase change becomes important part the code development procedure.

It is impractical and usually impossible to include all possible factors when modelling the environment numerically. In practice only limited set of data can be accessed and controlled experimentally. Most industrial problems involve configurations and substances which are very difficult to investigate experimentally. For example in case of modelling casting problems we find that metals and metal alloys are opaque, their melting temperature is very high and their physical properties are not known precisely enough. Hence, collected data is usually not sufficiently accurate to give a definitive answer on code reliability. One possible option is to use the so-called *analog fluids* which are transparent and have a low melting point. Such materials are most commonly aqueous solutions of salts, which crystallise with a dendritic morphology. Some organic liquids also lend themselves favourable to this purpose [13]. Experimental data obtained using simplified geometry and analog fluids may appear to be not sufficient to build confidence to reproduce all details of the practical environment. Nevertheless, our experience shows that before solving complicated problems industrial code should be able to reproduce properly also simplified configuration. And if there are problems found during such procedure, experimental feedback gained may appear valuable to improve the model.

A brief review of experimental techniques useful for the study of heat and mass transfer problems in the flow of liquid with phase change was given previously [13]. Applying them it is possible to construct properly planned experimental benchmarks for validating appropriate numerical codes. They may alert one to the sensitivity of the flow to the modelling simplifications, which would otherwise be hard to predict. As we have seen in our several attempts to build an experimental solidification benchmark using freezing water as medium [14–16] proper prediction of the flow structure is crucial. Hence, in the following we will discuss a simple configuration of differentially heated box allowing analysis of discrepancies between measured and calculated solidification experiments.

4. EXAMPLE OF THE VALIDATION METHODOLOGY

The proposed methodology to create an experimental benchmark we exemplify in the configuration which 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. It is obvious that the methodology described below contains factors specific for the particular problem. It solely gives an example of the procedure based on evaluation of experimental and numerical errors in purpose to estimate validation key metrics. Such metrics are necessary to evaluate accuracy of measured parameters necessary to find out to what extend the experimental benchmark can be used for the specific code validation. The validation procedure must be able to discriminate discrepancies caused by environmental variability, experimental and modelling uncertainty from those caused by parametric modelling errors. The inconsistency between the numerical model and the experiment must be assessed to permit its updating in the next step of analysis [16].

As we have demonstrated above the accurate solution of simple natural convection in enclosures already became a crucial task in a goal of achieving precise modelling. Additional complexity of the problem due to the phase change leads to new sources of uncertainties. Strong non-linearity of the coupled momentum and energy equations solved for two phases separated by moving boundary creates challenging task both for modelling as for accurate experimental monitoring of the phenomenon. Inevitable uncertainties in defining physical model result in serious discrepancies between numerical and experimental results encountered for a *simple* problem of ice formation in a differentially heated cavity. It motivated us to revise reliability and performance of typical solvers used for simulating heat transfer phenomena.

Before performing validation procedure it is necessary to estimate errors due to the numerical procedure. It creates need to formulate a 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 [12]. 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 (cf. Fig. 5). 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 was proposed. It is based on calculating deviation of the velocity and temperature profiles extracted along three selected lines crossing

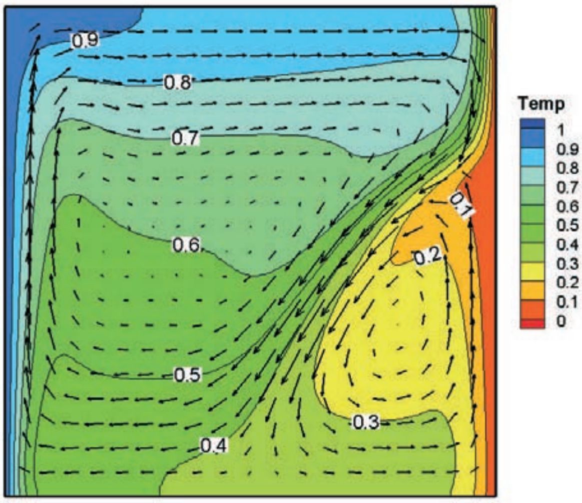


Fig. 5. Velocity field and isotherms obtained by simulating natural convection of water close to the freezing point in differentially heated cavity. Cold wall (right) kept at freezing point (0°C), hot wall (left) kept at 10°C. Density anomaly present at 4°C creates two counter rotating circulations close to the cold wall [12].

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.

The physical model used in the experiments differs in many details from idealised numerical benchmark. The natural convection of water was investigated in the differentially heated cube-shaped cavity made of Plexiglas. Finite conductivity of the wall material, its thickness and external air temperature in the lab define additional heat fluxes, necessary to be included in the model. The side walls kept at constant temperatures are made of metal. Cooling water from two thermostats is pumped through internal channels of the walls to assure their constant temperature. However, final thermal conductivity of the walls and limited heat exchange between coolant and the wall material produce uncertainty about degree of temperature uniformity and stability on the "isothermal" walls being in contact with fluid. 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 nonlinearities 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 which configuration is the least sensitive for changes in experimental conditions what significantly simplifies and helps in our laboratory investigations. Sensitivity analysis was conducted for the sake of boundary condition, initial condition and fluid properties. Based on our previous experience we took into account in our computational model not only fluid domain described in previous section but also both *"isothermal"* and *"adiabatic"* walls (cf. Fig. 7). The sensitivity analysis revealed that such a 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 (see Fig. 7) considerably changed the flow structure inside the fluid domain. The flow structure consisting of two counter-rotating circulations 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 simulation results with assumed constant values of viscosity, specific heat and thermal conductivity with those with variable fluid properties. It was found that variability of specific heat and thermal conductivity did not alter flow structure significantly, whereas variability of viscosity caused 8% decrease in velocity magnitude and has to be considered in the numerical model. The initial conditions 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 [18, 19]. Experimental set-up consists of cubic cavity with internal size of 80 mm, with two opposite side-walls made of a 14 mm thick aluminium, and four remaining walls made of a 8 mm thick Plexiglas. The

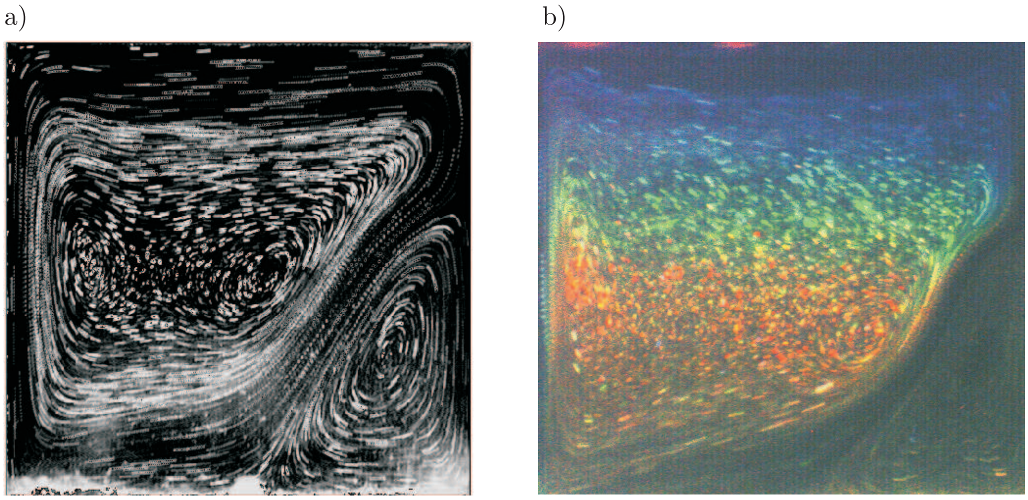


Fig. 6. Flow structure recorded for natural convection of water close to the freezing point: multi-exposed image of tracers used for PIV velocity measurements (a), temperature field visualised with liquid crystal tracers (b).

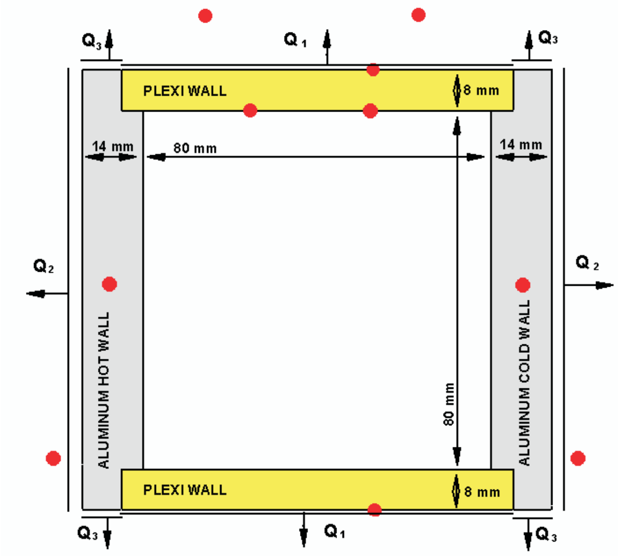


Fig. 7. Sketch of the physical geometry used in the validation experiment. Red dots indicate control points with point measurements of temperature.

left side aluminium wall was heated by coolant kept at the constant temperature $T_H = 10°\mathrm{C}$. The right side aluminium wall was cooled by coolant kept at the constant temperature $T_C = -2°\mathrm{C}$. It allowed to set internal cold wall temperature close to the freezing point 0°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 Fig. 7 (red circles). Steady state convection was assumed after running the experiment for several hours. 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 [13]. Figure 6b presents an experimental image of liquid crystal tracers changing their colour with temperature between 4°C and 9°C (red 4–6°C, yellow 6–6.5°C, green 6.5–7.5°C, blue 7.5–9°C). Pair of such images was used to obtained velocity field by PIV technique. Resulting 2D velocity and temperature fields are shown in Fig. 8. Additionally, temperature was monitored during the whole experiment in points depicted in Fig. 7 (red circles) by set of thermocouples. That allowed to estimate heat transfer coefficients necessary to calculate respectively heat fluxes Q_1, Q_2, Q_3 with required accuracy (for details see [19]).

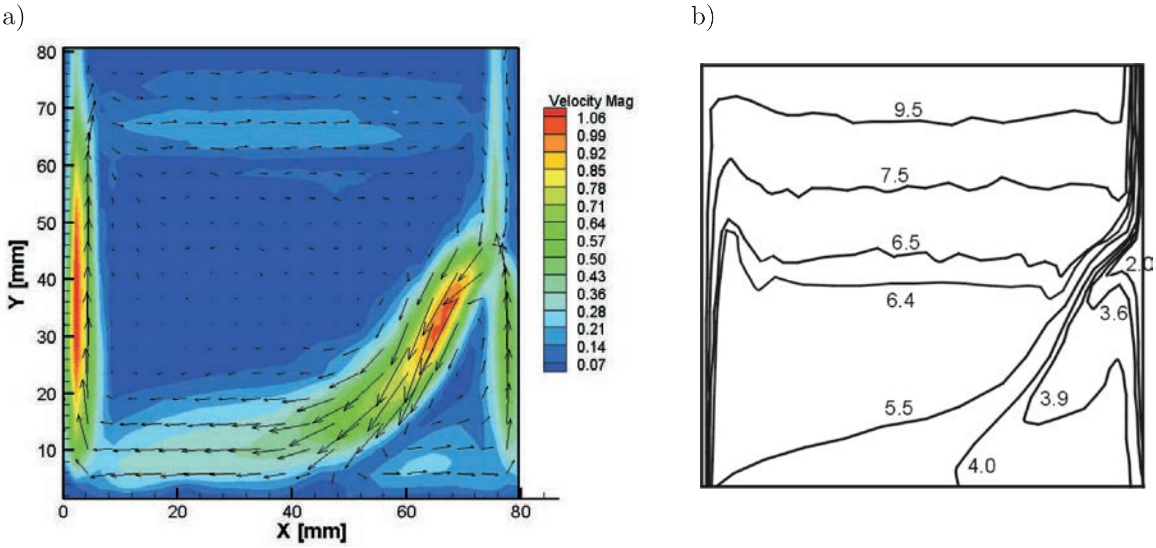


Fig. 8. Experimental data for natural convection of water close to the freezing point ($T_c = 0°\mathrm{C}$, $T_h = 10°\mathrm{C}$); a) velocity field measured (PIV) in the centre cross section coloured with the velocity magnitude contours; b) isotherms measured using thermochromic tracers [19].

Accurate experimental measurements allowed for application of appropriate boundary conditions into the previously verified computational model. Finite volume code Fluent [20] 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 Fig. 9.

To estimate validation metrics we have to analyse errors originating from the simulations and due to the experimental uncertainties. The simulation error includes relatively easy to estimate errors due to the limitations of numerical procedure and more difficult to estimate *a priori* modelling errors. To estimate modelling error we have to compare sequence of simulation results with the experiment. Defining difference of between numerical and experimental model for selected parameters and relating it accuracy of measurement, we construct functionals describing sensitivity for each of them. For simplicity we limit our analysis to stationary flow, hence deviations of initial conditions both in the numerical as in the experimental case are neglected. Experiments, described already

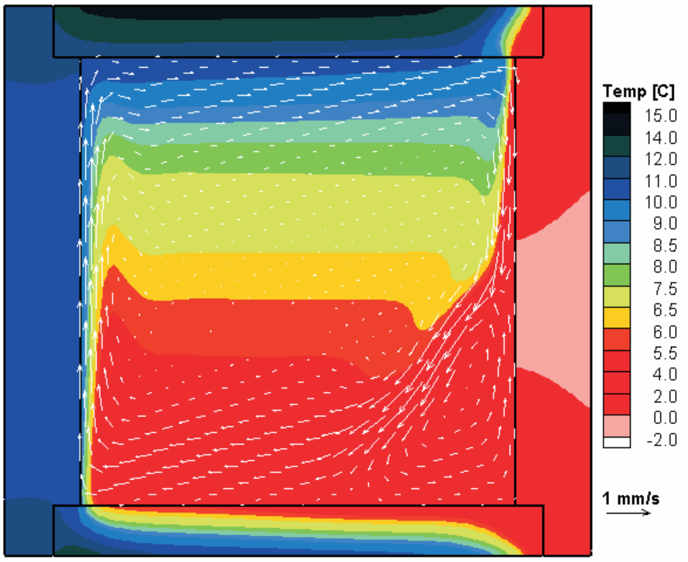


Fig. 9. Velocity and temperature fields computed for *physical* configuration, used for the code validation procedure. Nonuniformity of temperature is clearly seen both for *"adiabatic"* as well as *"isothermal"* walls [19].

before, indicated importance of the thermal boundary conditions for natural convection in the cubic cavity. Proper implementation of these conditions depends on details of the numerical model applied for the walls. Hence, several versions of the numerical codes were applied modelling heat fluxes within more or less extended description of all six walls geometry and their thermal properties. The experimental errors considered are uncertainties of temperature measured at 10 points (external, within bounding walls and internal), uncertainties of material properties (viscosity, density, thermal diffusivity) for fluid, isolating walls (Plexiglas) and isothermal walls (aluminium). The flow and temperature fields are obtained form the experiments with uncertainties of measured temperature isotherms (colour analysis of thermochromic tracers), and uncertainties of measured velocity fields (Particle Image Velocimetry). For each component of the uncertainty analysis the simulations were performed changing value of the parameters within the range of uncertainties. The result of these simulations gave us large matrix of possible deviations of velocity and temperature fields due to the experimental uncertainties of the defined benchmark flow. From these tests it must be concluded that not all elements of the matrix fulfil validation condition, which says that validation is valid only if the experimental uncertainty is below deviation from the numerical result [19]. Therefore, experimental validation of the numerical code is limited by sensitivity of the flow to the data uncertainties. In the particular flow with natural convection of water close to the freezing point, the most sensitive to modelling errors appears the flow region close to the cold wall. As this region decides about initiation and propagation of the freezing front, it is crucial to look at the velocity structure closed to the cold wall when validating results of the numerical models used for solidification problems.

5. Conclusions

In many areas of Computational Fluid Dynamics, numerical models are developed for predicting the response of a system when the phenomenon is not accessible by direct measurement or when numerical simulations are cheaper than experiment. Nevertheless, developing more or less sophisticated models does not necessarily guarantee accuracy and predictability. The plethora of assumptions and simplifications involved in successive steps of idealization and discretisation of the physical world yields numerous sources of discrepancies of the modelling predictions. The total predictability that may be expected from a particular model depends on the purpose intended for that model. Traditional approach for model testing is limited to a single effort of reproducing the test data with adequate accuracy. This does not guarantee predictability away from the region of modelling that relates to the test data. Also, this approach may be irrelevant if experimental data are not accurate enough to provide deterministic output. Here, we have shown example of methodology allowing to estimate parameters necessary to perform model validation and to determine major sources of uncertainty which must be accounted for to fully capture the range of variability of the systems analysed. We conclude that the concept of model validation should be strongly coupled to uncertainty quantification, a relationship that has generally been overlooked by the conventional testing trustworthiness of CFD models.

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