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The numerical simulation of buoyancy-induced transport processes.

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Introduction

Annex 20, under the heading of "Air Flow Patterns", proposed to evaluate the performance of single- and multi-zone air and contaminant flow simulation techniques and to establish their viability as design tools. Belgian research groups were active in this task, by producing a great deal of experimental work.

At the very time when it is reaching completion, the experts involved in this program develop the idea, among others, for a new annex on the so-considered "hot" topic of "Energy, Air and Contaminant Flows within Large Enclosures", while annex 23 centres future interest upon "Multizone Airflow Modelling".

This selection of closely connected research areas, from international specialists in energy management, obviously emphasizes the absolute need for a better understanding of air movement, heat and mass transfer within rooms, as they are responsible for the thermal comfort and the air quality in the indoor environment, for the ventilation effectiveness and the optimization of energy consumption in the buildings.

Computer simulations rank among the possible techniques for clarifying the characteristics of indoor airflows and convected pollutants. The strengths and limitations of numerical methods in ventilation design were evaluated in annex 20. The results of numerical exercices are presently being critically reviewed. At the moment, we are unaware of the inferred conclusions, as we were not personally involved.

Our purpose will therefore reflect our feeling from individual experience and will tentatively suggest useful recommendations and new ideas for improving the numerical prediction of buoyancy-induced transport processes.

The physical features of a complex flow pattern

Air movements in buildings range among the internal flow problems partially or totally induced by buoyancy-driving forces. Fluid motions an transport processes generated or altered by buoyancy are extremely complex.

In confined natural convection flows, boundary layers develop alon the walls and encircle a core region which, therefore, cannot be determine from the boundary conditions. The flow pattern in the central region depends on the boundary layer and this latter, in turn, is influenced by the cor wherein distinct and multiple flow subregions may quite often be imbeddec This interaction, inherent to all confined convection configurations invalidates the classical boundary layer theory and prevents from usin its relevant results. As proven by experience, the high sensitivity of thi coupling to changes in the container geometry and in the prescribed boundar conditions makes hazardous any use of data from seemingly similar problems.

It should moreover be remained that two basic modes of flow are essen tially generated by buoyancy. The first one occurs whenever a densit gradient is normal to the gravity vector ; a flow ensues immediatel referred to as conventional convection. The second mode occurs when density gradient is parallel but opposed to the gravity vector ; the flui remains, in this case, in a state of unstable equilibrium until a critica density gradient is exceeded and induces a spontaneous flow of cellula like structure. If the density gradient is parallel and in the sa direction as gravity, the fluid is stably stratified. Both conventiona and unstable convection can of course interact, and actually do in mo practical building applications.

As if all that was not difficult enough to deal with, the air fl is locally or completely turbulent in rooms of standard dimensions, und the smallest temperature differences, as the interaction between the fl and the driving force alters the regions in which the buoyancy acts.

The complexity of the phenomena and the large diversity of natur convection problems keep on posing challenging physical and mathematic interrogations, ignored or unanswered through the existing literature. Th lack of understanding looks particularly crucial for working out integr models, suitable for running in large computer simulation models of t thermal environment in building science. In constant development, includi the most sophisticated solutions of certain well-known diffusion and radi tion transfer processes, taking into account the utmost internal gains and the smallest infiltrations that may influence the comfort, the indoor air quality or the energy consumption, all of these programs cavalierly consider each constitutive space as an isothermal volume, with a single, and otherwise debatable, central temperature. This crude assumption obtusely ignores the fundamental momentum conservation principle, responsible for the afore-mentioned coupling of the boundary and core flows, the interaction between the flow and the driving force and the occurence of flow subregions.

A critical review of computational predictions

The experimental work on natural convection in enclosures has usually been critical in revealing the true nature of the flows, in providing unforeseen aspects with important insights, in indicating the folly of early physical hypothesis for such complex problems. It has produced lots of data, commonly compiled in the form of correlation laws of the recorded measurements, for numbers of complicated engineering applications that would otherwise have remained undocumented. It will continue to serve the design of numerous technical projects and will definitively remain essential for guiding and validating any further analytical or numerical research.

It may indeed be thought, and the author shares the opinion, that the cost effectiveness and the greater flexibility of computer simulations will allow them to play an increasing role in building design, whereas field tests are becoming impractical, time-consuming and expensive. It may as fairly be considered, on the contrary, that the available numerical data for confined buoyancy flows in basic configurations are still questionable enough to deny or delay the reliable predictive capabilities of computational techniques in solving actual thermal convection influenced problems.

The upholders of this latter thesis certainly have several arguments to advance, as it should be conceded that there has been no truly trustworthy numerical results of velocity and temperature distributions in buoyancy-driven flows, for a long while. The inserted two first figures show the available data from analytical, computational and experimental means, as they could be compiled some years ago, in relation with one of the most investigated relevant problem, i.e., the two-dimensional air flow in a rectangular enclosure between vertical isothermal walls at different

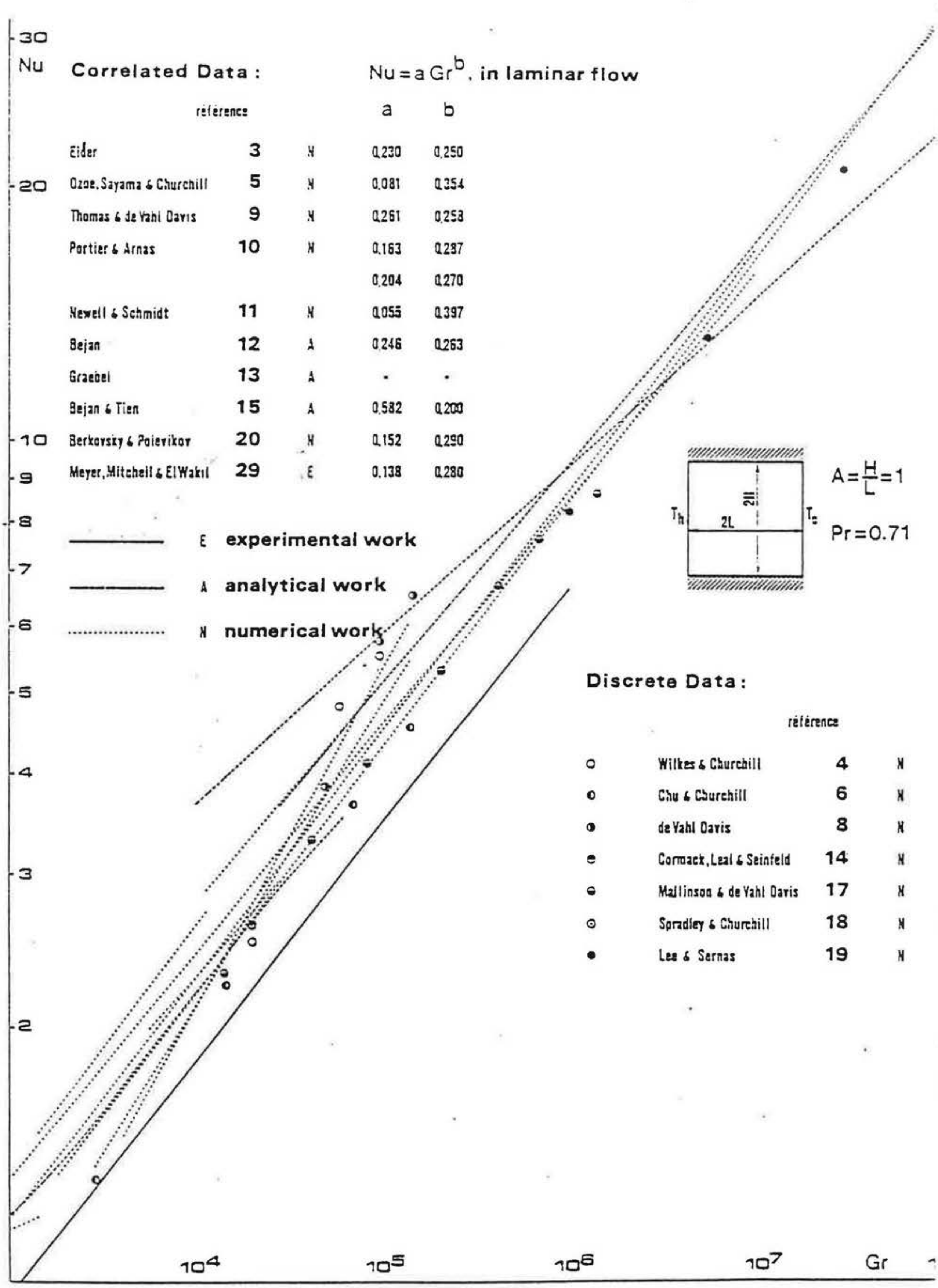
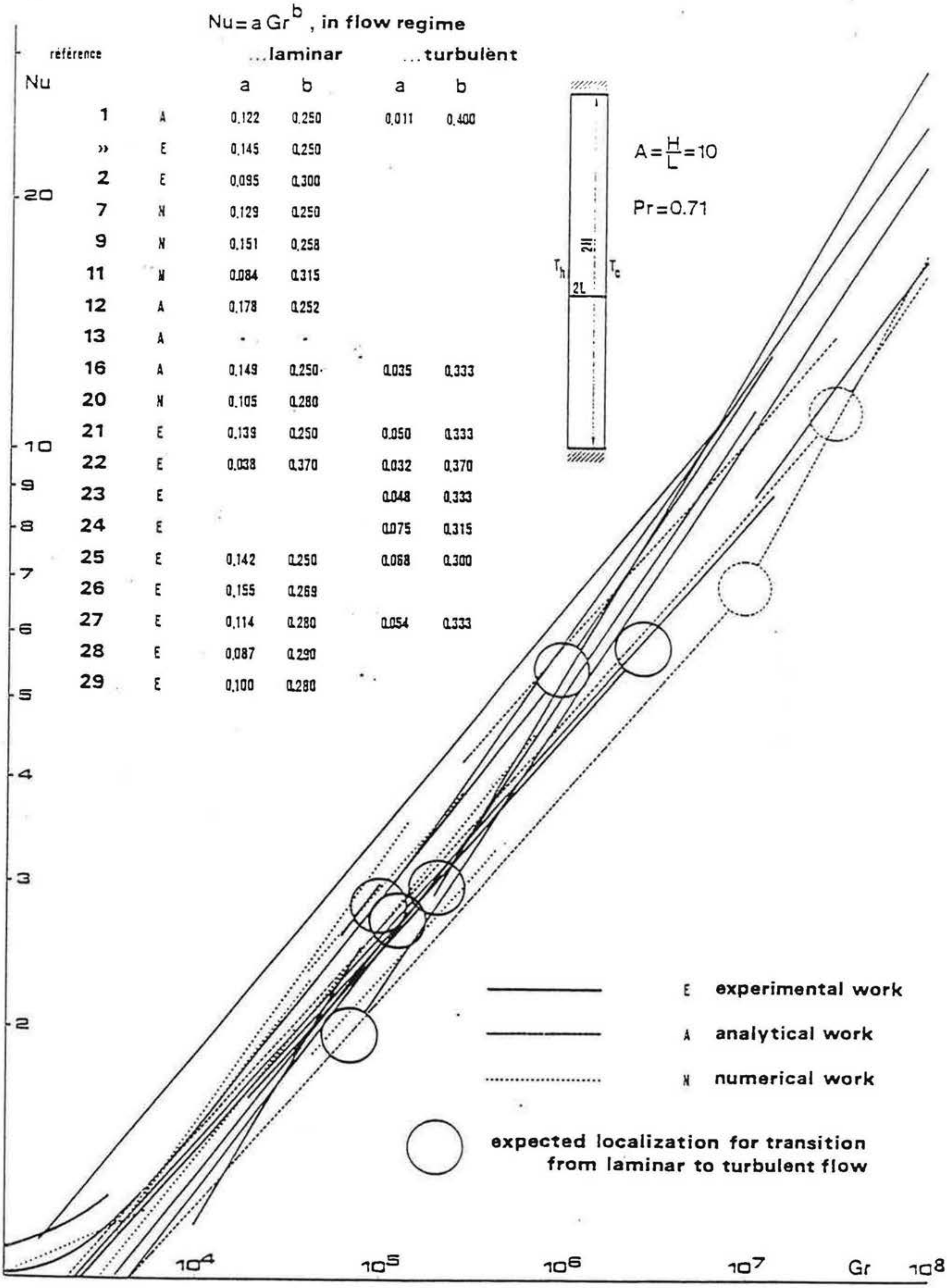


Figure 1 : A survey of mean Nusselt number estimations
for natural convection in a square cavity.



référence		...laminar a	...laminar b	...turbulent a	...turbulent b
1	A	0,122	0,250	0,011	0,400
»	E	0,145	0,250		
2	E	0,095	0,300		
7	N	0,129	0,250		
9	N	0,151	0,258		
11	N	0,084	0,315		
12	A	0,178	0,252		
13	A	-	-		
16	A	0,149	0,250	0,035	0,333
20	N	0,105	0,280		
21	E	0,139	0,250	0,050	0,333
22	E	0,038	0,370	0,032	0,370
23	E			0,048	0,333
24	E			0,075	0,315
25	E	0,142	0,250	0,068	0,300
26	E	0,155	0,269		
27	E	0,114	0,280	0,054	0,333
28	E	0,087	0,290		
29	E	0,100	0,280		

Figure 2 : A survey of mean Nusselt number estimations for natural convection in an elongated cavity.

temperatures, with horizontal boundaries being kept adiabatic. The comparison is reported for the values 1 and 10 of the aspect ratio. The spreading of the predicted heat transfer, in the form of the Nusselt number in terms of the Grashof number, reveals the extent of the discrepancies between the proposed formula in laminar flow ; the inferred location of the transition regime makes any comment needless and the turbulent flow range is itself quite undocumented. As a matter of fact, our understanding was no more than a crude picture of a phenomenon in obvious relation with building physics, but also considered as highly essential for reactor insulation, cooling of radioactive waste containers, fire prevention, solar energy collection, dispersion of waste heat in estuaries or cristal growth in liquids.

At the same period, numerical contributions were invited to the solution of the same problem in a square cavity, proposed as a suitable vehicle for testing and validating computer codes. For air, with a Prandtl number of 0.71, the flow and thermal fields were expected up to a Rayleigh dimensionless parameter, product of the Grashof and Prandtl numbers, of 10^6, far below the required range for most of the actual applications. With common reference scales, a quantitative comparison was planned on the basis of definite values of specific quantities, such as the average Nusselt number, its maximum and minimum local values along the vertical walls, and the maximum vertical and horizontal velocity component in the boundary layers on the respective horizontal and vertical midplanes. Figure 3 collects the twenty-seven significant estimates for these quantities, out of thirty-six contributions received from nine countries ; they are compared to what was claimed the best available solution, obtained through a Richardson extrapolation of the results computed with successively finer meshes, up to eighty-one grid points in each direction. At the only sight of the recorded divergencies, it clearly appears that the exercise could not serve as the expected assessment of computational algorithms, but merely confirmed the limitations of numerical fluid dynamics in producing, at that time, reliable predictions of buoyancy-induced flow and heat transfer.

Lack of progress in the numerical simulation of natural convection can be attributed to several reasons, the understanding of which may induce thoughtful and efficient counter-remedies.

- The first one is related to proper normalization of the equations, referred to as dimensional or scaling analysis. It is disturbing to note that the constitutive equations have rarely been normalized, i.e., not only been made dimensionless but also of unit order of magnitude. The result is that the dimensionless parameters, which appear as coefficients of various terms, do thus not properly indicate the relative magnitude of each term. The large parametric values associated with natural convection problems cause the terms to have disparate magnitudes, that can lead to considerable numerical difficulties and even to misrepresentation of the proper physics.

In almost every numerical paper in the literature, the velocity is made non-dimensional, not normalized, by using the viscous velocity. As a consequence, the Grashof or Rayleigh number appears as the coefficient of the buoyancy term. Since these parameters have values on the order of 10^4 to 10^8 for laminar flow, the buoyancy force is made the dominant term in the equations. There are, however, regions in which there is no buoyancy, such as the core for boundary layer flows, but a very small numerical error in the buoyancy term can cause it improperly to contribute to the solution there and, thus, misrepresent the true physics.

- The second reason arises from the used mesh or element size in the immediate vicinity of the rigid boundaries. With too few node points, if any, across the adjacent viscous and thermal layers, the numerical simulations cannot but sketch roughly the boundary flow and, therefore, ignore its interaction with the core, which has been emphasized as a crucial aspect inherent to natural convection in confined configurations. The resulting hazy accounting for the characteristic coupling between the flow and the buoyancy-driving force makes it difficult to avoid skepticism of purely numerical solutions. Most certainly, it should nevertheless be admitted that the too coarse discretization of the continuum is required by storage limitations and computing time restrictions.

To give credence to the numerical results, the calculations are usually compared to others, subjected to the same critical remarks, or to such experimental data as the average Nusselt number. This last is however a gross parameter, which is generally insensitive to details in the velocity and temperature distributions, so that the indicated agreement does not ensure the correctness of the computed fields at all. The insensitivity for flow analysis. On the other hand, the solution techniques for handling the coupling between the momentum and continuity equations will not be explicitly included in our consideration, as they dictate the efficiency of the algorithm without altering the final computed fields, if stability requirements are satisfied.

It would be useless to remove the acknowledged criticizable features of the numerical simulation of confined natural convection problems with appropriate alternatives, if the availability of a turbulence model is not established ; this is, of course, of capital importance for any practical application in building physics. The matter remains an extensive field for fundamental and applied research, as the physical understanding of the phenomenon is itself far from being acquired. It should however be admitted that useful, though improvable, tools have been developped and widely tested for ensuring a realistic representation of most of the arcana of turbulence. The adjunction to the continuity, momentum and energy equations, for the primitive variables, of the transport equations for the turbulent kinetic energy, the rate of its dissipation and suggestively, the square of the temperature fluctuations makes up a closed differential system for a reliable and detailed description of turbulent flow and heat transfer. Specific models, inclusive of buoyancy-driving forces, have been proposed and discussed elsewhere and will not be reproduced here.

- The correct scaling of the constitutive equations is easily obtained, if particular attention is paid to this important problem. The normalization of natural convection problems has clearly and explicitly been delineated. Let us just recall that, whenever velocity and thermal boundary layers exist in air, the reference velocity should be taken as $\frac{\nu}{L}(Gr)^{\frac{1}{2}}$, in terms of the viscous velocity and the Grashof number, because no velocity scale is imposed in buoyancy-driven flows.

- The second afore-mentioned weakness of most of the numerical calculations of natural convection in confined configurations is also easily removed. The discrete representation of the boundary layers should include enough node points across their thin thickness to ensure a faithful description of their actual physical pattern and give credence to the simultaneous simulation of their interaction with the enclosed core flow. The grid refinement in the boundary regions is all the more essential as first-order approximations of the convection fluxes are required in these layers with high velocity and temperature gradients, on account of numerical stability of the calculations. Care must also be taken if an irregular discretization of the physical domain is made uniform in a computation volume by changes of the space coordinates, as the difference analogs of the transformed differential equations correspond to down-graded approximations of the original system in the physical model.

Concurrently with the advent of supercomputers, all of these requirements may, at present, be handled satisfactorily and should be treated accordingly, so true is it that a coarse discretization of the boundary regions cannot but lead to meaningless results in the entire flow field.

The difficulty of finding the proper mesh may still hold in the core itself, if no a priori information exists on the flow pattern, for indicating the occurence of unexpected or unusual aspects such as flow subregions. The use of local gradient detectors may prevent from any misrepresentation by inducing an automatic grid refinement to find the required resolution thereabout. This computational facility is of importance for improving the numerical predictions and its request has to be considered from the selection of the general solution algorithm, that it may influence.

- By nature, the third argument, objected to the reliability of purely numerical solutions, is much more fundamental ; its adjustment has not been improved through the very substantial progress of the solution techniques in recent years and cannot be expected from the development of vector- and parallel-processing capabilities. The formulation of a satisfactory convection scheme remains an unresolved question in computational heat transfer. The lower-order methods such as upwind or hybrid produce bounded and apparently realistic solutions, but involve significant false diffusion likely to question their very meaning. The methods proposed for the elimination of false diffusion have negative influence coefficients, produce non-physical overshoots and undershoots and lead to oscillations and divergence at high flow rates.

The asymmetric nature of convection is recognized and should relevantly be reflected in its discretization scheme. So-called flux-vector splitting or flux-difference splitting algorithms and upwind discretization schemes of suitable accuracy of the convection fluxes are presently being developped, in relation with computational compressible fluid dynamics. Their extension to viscous incompressible fluid flow model is quite straightforward. In principle, the flux-vectors or differences of flux-vectors are decomposed in a sum of two terms, so that their individual jacobian matrix has real eigenvalues with the same sign ; once this decomposition is achieved, each part of the splitted space gradient is treated by a different difference stencil, adapted to the direction of propagation. Several formulations are well-known already, associated with the names of Steger and Warming, Van Leer, Roe, Osher, ... Contrary to most of the previously used upwind schemes, all of these splitting methods have achieved a high degree of sophistication and understanding. The still questionable subjection of the available decompositions to rather arbitrary mesh dependent directions in multi-dimensional configurations is being corrected by purely flow dependent intrinsic alternatives.

The inferred formulations of the convection terms are easily implemented on any kind of structured or unstructured polyhedral meshes. The corresponding discrete approximations can be made second order accurate, without any false diffusion, even on strongly stretched and skewed grids. The use of suitable limiters may be recommended for switching in a continuous manner to first order schemes to avoid the oscillations that could appear in regions with sharp gradients.

Concluding remarks

The number of required improvements in the available numerical techniques does not diminish what has already been solved, nor do the prospects of successful simulations reduce the importance of experimental research.

The main shortcomings in the usual numerical treatment of natural convection problems have been identified and proposals have been outlined for their solution, by taking advantage of the simultaneous and most recent advances in computational fluid dynamics and in computer hardware.

On these basis, it is felt that the numerical simulation of buoyancy-induced processes could achieve the required accuracy and reliability of its predictions, while extending the upper limit of its computational capabilities. Physical insight into complex patterns, in relation with practical problems, could be thought about in terms of computational analysis. As in other industries where numerical techniques are vigorously used, heating, ventilating and air-conditioning applications could benefit by a better understanding of their leading transport agent to improve the energy management programs, to predict air movements in buildings, to objectify comfort analysis and to determine the distributions of pollutant concentrations for indoor air quality.

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