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Discussion Note

Summary The validation of computer predictions of physical processes is still a topic of concern, particularly in relation to dynamic thermal simulation modelling. However, far more complex computer programs are now being introduced into the building services industry. These new programs solve the conservation equations of momentum, energy and mass to simulate air movement in and around buildings. The validation task is potentially more difficult than that encountered to date. This paper discusses some of the problems associated with the application and validation of these codes and suggests how a user can ensure that the physical processes are being modelled realistically.

How accurate are the predictions of complex air movement models?

M J HOLMES† BSc ACGI DIC MCIBSE and G E WHITTLE‡ MSc PhD CEng MIMechE

† Arup Research and Development, 13 Fitzroy Street, London W1P 6BQ, UK

‡ Building Services Research and Information Association, Old Bracknell Lane West, Bracknell, Berks RG12 4AH, UK

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The use of complex computer based dynamic thermal models in the analysis of buildings and their systems is slowly becoming an accepted part of the design process. This is happening despite the limited availability of supportive validation reports on the programs used(1). The methods of calculation are often not understood by the user, or can in some cases be no more than an adapted hand calculation method, but for which the computer code and detailed model documentation are not available for inspection. It would seem necessary therefore for the user to have considerable faith in the author of the program—who may well be a brilliant theoretician, but with little practical engineering experience. However, in practice the user normally has a wealth of experience-based knowledge to assist him in the interpretation of the output. In addition where systems are concerned it will usually be apparent if unrealistic or improbable operating conditions are predicted. Where unexpected conditions are predicted, there will (or should be) more doubt as to the validity of the output—it may or may not be correct.

A new thermal model has now arrived, for which it is doubtful whether many users will have sufficient experience in judging the validity of the results, and it is almost certain that they will not understand the theoretical basis of the method. This is the numerical air movement model.

The main application of this model is in the study of room air distribution, that is, being able to predict air movement patterns and temperature gradients within a room or enclosure. An understanding of air distribution at the design stage is important for achieving appropriate levels of thermal comfort, air quality, or for controlling contaminant levels in a process area. Within a given space air movement is governed by the magnitudes of supply air momentum and convective heat release to the air. Except for very simplified cases which are covered by design guidance information, there are no easy ways of judging the likely acceptability of various design options. In the past, where a proposed system was of novel design or where confidence levels needed to be increased, physical modelling in the laboratory was the usual course of action. This approach can be quite time consuming and therefore costly, involving the construction of a test module and the demonstration and optimising of the air movement conditions. Now, with the development of numerical air movement models there is the possibility, in certain cases at least, of being able to analyse design options using computer methods, and at a much reduced cost.

Air movement, or more strictly, computational fluid dynamics codes have been with us for some time(2). At present their use is fairly restricted because of the computer power required, although new developments in hardware are changing the situation. The attraction of these models is that they can predict two- and three-dimensional air velocity and temperature fields within any defined enclosure. Colour graphics can be employed to enhance the output, which may be in the form of velocity vector and temperature contour plots. There are facilities available to make the output look like measured results from a real building—but how real are the predictions?

It takes little knowledge of engineering to know that the more complex a machine the more likely it is to fail through shortcomings in design. The same applies to computer programs. Unfortunately the program will usually continue to work but the answers may be incorrect. The only way to ensure that the answers obtained are correct in the sense that they represent a true solution of the flow field defined by the input data (the often used statement 'garbage in, garbage out' also applies here) is to carry out some tests. This note proposes a suitable set of tests based on the present 'state-of-the-art' of the codes.

Computational fluid dynamics (CFD) codes operate by solving the fundamental conservation equations of momentum, energy and mass. These are partial differential equations which represent convection and diffusion processes; they are very complex and cannot be solved analytically in the same way as conventional equations. The way forward is to adopt numerical analysis techniques. The most widely used approach is the 'control volume' formulation[3,4]. Firstly, the flow domain (the space bounded by the inner surfaces of the room or enclosure) is overlayed with a flow mesh comprising many small 'control volumes'. Control volumes, termed flow cells, are small volumes of space which collectively make up the room or enclosure. Each differential equation is then expressed in 'difference' or 'discretised' form so that the value of a variable within a flow cell is expressed as a function of variable values within surrounding cells. Neglecting at this stage the need for a turbulence model, the variables comprise the components of the velocity vector (two or three), temperature and pressure. The 'difference scheme' used to generate a numerical approximation of the differential equations should ensure that the fluxes of momentum, energy and mass over the boundaries of the flow cells together with any sources (or sinks) within individual cells are conserved. Hence, the partial differential equations are approximated by linear algebraic equations which can then be solved using fairly conventional numerical procedures. Unfortunately, because of nonlinearities in the initial equations an iterative solution sequence must be adopted; the equations are repeatedly relinearised and solved until the solution is reached. This is computationally very intensive and places a major demand on computer facilities.

Turbulence modelling is an important consideration since in almost all air movement problems of practical interest the flow regime is turbulent. The most widely used turbulence model is known as the *k*–epsilon model[5]. This, in simple terms, consists of a set of two equations, one for *k*, the kinetic energy of turbulence, and one for epsilon, the rate of dissipation of turbulence energy. They are both represented by convection–diffusion equations of a form similar to those which describe the conservation of momentum and energy. They are solved in a similar way by repeatedly discretising the differential equations and numerically solving the resulting linear algebraic equations. Despite the fairly widespread application of the *k*–epsilon model it is still semi-empirically based, requiring the use of a number of experimentally determined constants. It also significantly increases the computational requirements and may at times be responsible for delaying the convergence of the equation set to a solution. Other simpler models of turbulence can be used to good effect in certain applications. However, it is not proposed to discuss these here.

The accuracy of numerical air movement codes depends not surprisingly on many factors. These can be categorised under headings associated with the specification of the boundary conditions, the selection of the location and number of flow cells, the discretisation scheme, the turbulence model used, and the convergence criteria adopted for terminating the iterative solution sequence.

The boundary conditions comprise information about the geometry of the room including the position and shape of any major physical obstructions within the space; the location of supply and return air terminals and the velocity, flow rate and temperature of the supply air; a specification of convective heat transfer (or surface heat transfer coefficients) from/to the surfaces of the room, and any convective heat release into the space from occupants, equipment, lighting and solar gain. The physical boundary conditions (shape and finish) all influence the final result and so should be modelled realistically.

The accuracy and economy of the calculation is influenced strongly by the specification of the flow mesh on which the equations are solved. For accuracy it is necessary to concentrate cells in areas of the flow field where steep variations of velocity components or temperature are expected[6]. For example, such areas would be those close to supply air terminals, and surfaces of the room, particularly those at which convective heat transfer is taking place. Any loss of accuracy by specifying too few flow cells will not be obvious unless further computations are performed at greater mesh resolutions. When dealing with three-dimensional flows in a consultancy environment the computer resources and costs at the present state of hardware development will be stretched to the limit. The number of flow cells required for a three-dimensional calculation will probably be in the region of 4 000 to more than 10 000, and the computer time required increases nonlinearly with the number of cells. Rarely will it be possible, other than in research applications, to undertake mesh sensitivity analyses in three-dimensional flows. A way around this difficulty is to simplify a three-dimensional problem to one of two dimensions, the latter representing the main features of the full problem. Sensitivity analyses can then be undertaken much more readily. When an appropriate resolution is found then the problem must be translated into its full three-dimensional form to generate the final results. Consistency of mesh resolution in the third dimension must, of course, be retained.

The discretisation scheme most commonly used in control volume methods is the hybrid difference scheme, which combines upwind and central differences. It is claimed that this scheme provides the best compromise between good convergence characteristics and accuracy[4]. A flaw in the scheme is that the locally one-dimensional treatment of the convective flux leads to a false (numerical) diffusion under conditions where streamlines and mesh lines are steeply inclined. This manifests as an artificial and unrealistic enhancing of viscous effects. The remedy, at present, is to increase mesh resolution, although other schemes are under development which may well overcome this limitation soon[7].

As already stated, the turbulence model can have a major impact on the way the calculation proceeds, and on the solution. Very often the user of the code will be at the mercy of the CFD expert since this area of development is very complex.

Since these calculation methods are iterative some judgement needs to be exercised as to when to terminate the solution sequence. This is necessary since the rate of convergence to a solution reduces as the solution is approached. For the sake of economy of computer time the calculation is usually stopped when the sums of the residual fluxes of momentum, energy and mass in the flow cells reduce to an acceptably low level. The residual fluxes represent the magnitude of error in the current solution of the equations. It is important that convergence criteria, applied in terms of residual fluxes, be related to the total inflow or transfer of flux across the boundaries of the flow field. Information on the flux residuals should be printed by the code at the end of each iteration. While they do give an indication of the extent to which the numerical representations of the equations have been solved, it is also useful for the user to do some elementary sums to verify that mass and energy have been conserved in global terms; that is, that the mass outflow across the boundary matches the inflow and that the heat pick-up in the ventilation air equates to the heat release within the space. Also, it is often possible to apply simplified tests to, for example, establish from the output of the code the predicted velocity decay or trajectory of a supply jet and compare with experimental data obtained under similar circumstances. If there are significant inconsistencies then the reasons for these should be examined.

In summary, it is recommended that when using numerical air movement codes the user undertakes the following steps to ensure that accurate and good quality results are obtained:

(*a*) The problem must be specified accurately in terms of the boundary conditions: geometry, air velocity (and implied mass flow rate), air temperature, convective heat transfers across boundaries and other convective heat release in the space are all vitally important and, collectively, they specify the problem uniquely.

(*b*) Wherever possible, previously obtained experimental data or validated numerical results should be drawn on to give confidence in the approach being adopted, and also in the general validity of the findings.

(*c*) In the event of a lack of supporting evidence from previous similar exercises, a sensitivity analysis should be carried out to ensure that the resolution of the flow mesh is not influencing results. If necessary, the sensitivity analysis may be undertaken in a two-dimensional flow model provided it represents the main features of the three-dimensional case. Once the appropriate resolution is attained then the analysis should be repeated using the three-dimensional model to generate the final results. The resolution of the mesh in the third direction should be consistent with the two-dimensional case.

(*d*) The convergence criteria, expressed in terms of the residual fluxes, should properly reflect the level of accuracy required. Typically, convergence criteria expressed as 1% of total momentum, energy and mass transfers across boundaries would, in most cases, be appropriate.

(*e*) The user should ensure that mass and energy are conserved globally cross the boundaries of the flow field. In many cases this is a simple task but one which can be very informative.

This brief, critical review of the accuracy of numerical air movement codes should be seen in the context of promoting their proper use in the analysis of design options. For this purpose they provide a powerful computational tool but one which must be used with care and caution; the exercise of engineering judgement is of paramount importance.

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