

Thermo-fluid analysis in the built environment: expectations and limitations

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SYNOPSIS - Since the late 1970's, advanced computer models have been developed for the prediction of air flow, field temperature and pressure distributions, smoke (or other contaminate) dispersion, in the context of the built environment. These models are based on the established numerical techniques known as computational fluid dynamics (CFD). The complex nature of CFD models has made them far more difficult to use than the CAD and HVAC software tools currently used by architects and building services engineers.

The need for building and environmental microclimate analysis (using CFD calculation methods) is outlined, together with the capabilities, limitations, costs and userfriendliness of computational fluid dynamics software.

NOTATION

a	coefficients in discretization equations
C	convective term in discretization equations
D	diffusion term in discretization equations
k	turbulence kinetic energy (m^2s^{-2})
S_ϕ	sources or sinks of variable ϕ
S'_p, S''_p	coefficients in linearised sources or sinks in discretization equations
t	time (s)
u_j	time-averaged velocity components in the coordinate direction x_j ($m s^{-1}$)
x_j	coordinate directions (m)
ϕ	any dependent variable
Γ_ϕ	effective diffusion coefficients for each ϕ
ρ	fluid density ($Kg m^{-3}$)
$\alpha (I_{Pe_n})$	weighting function
p and n	indices, denoting respectively, central and neighbouring nodes in domain discretization grid

1 INTRODUCTION

In recent years, advances in computer-aided engineering design have been accompanied by a proliferation of applications in the built environment, notably in architectural design and structural analysis. Since the mid-1970's a number of sophisticated dynamic building energy simulation programs have been developed, which are now being taken up by the building industry. Those for computational fluid dynamics (CFD), however, have moved relatively more slowly. The reason for this is that the mathematical representation of the physics of fluid flow, and the numerical solution procedures used in CFD models are far from simple.

The author and his co-workers developed a range of thermo-fluid calculation methods for determining air flow and convective heat transfer in and around buildings over the period 1980-1986. The emphasis was placed on meeting the needs of thermal simulation programs for accurate input data in convective heat exchange in and around buildings. The calculation methods ranged from 'lower-level' approaches, including analytical solutions and elaborate data correlations for limiting cases (see, for example, (1)), to the development of a 'higher-level' flow model, using CFD techniques to the solution of the governing partial differential equations for microclimate analysis of building enclosures (2). This program, known as the ESCEAT (Elliptic Equation Solver for Convection and Heat Transfer) code. Both the lower and higher-level models have been used to develop and verify 'intermediate-level' computer codes, which formed the basis for generating input convective heat transfer data for dynamic building models (3) and (4).

In the present contribution, the environmental and building services requirements for predicting airflow and related phenomena, such as convective heat transfer and smoke movement, in the context of the building environment are outlined, together, with the capabilities, limitations, costs and userfriendliness of the current CFD software for microclimate design of buildings.

2 BUILDING AND ENVIRONMENTAL PERFORMANCE ANALYSIS

Industry and commerce have evolved stringent needs for environmental control which demands ever more sophisticated design methodologies. Design issues, such as energy consciousness, thermal comfort, environmental quality and hazard have produced demands for change of building design in order to reduce their negative impact on energy consumption, human comfort, safety and the "green" environment. These are largely influenced by the thermal behaviour of the buildings structure and air movement in and around buildings.

Predicting the actual energy consumed by a building is a complex function of prevailing climate influences, environmental requirements, building fabric, plant and control systems. In the last decade it has become increasingly recognised that in order to develop realistic methods for energy-conscious design of buildings it is necessary to model the dynamic energy performance of the system (5). These dynamic models require a computational solution, in contrast to the manual-calculation methods used with the traditional steady-state procedures. Thermal models are capable of providing the detailed information necessary to configure effective solutions for thermal design and management of buildings. However, a weakness in these models is that the emphasis has been placed on dynamic thermal performance of the fabric, while airflow and convective heat exchange in and around the building are modelled using only rough approximation (4). In addition, they provide only an averaged space air velocity and temperature, rather than the field values of these variables, which are required for thermal comfort and safety assessment of the environment.

In recent years, the need for environmental quality and hazard analysis within building spaces has taken a high profile in the design and maintenance of controlled and acceptable environments. This need has been particularly amplified by the adoption of features such as atria in building complexes, passive solar buildings and complex shopping centres which create further dilemma in the prediction of airflow and temperature distribution. Until recently, the only methods for obtaining a realistic prediction of the air/smoke movement, temperature and pressure distribution in and around buildings were to perform field measurements or to use models in wind-tunnels. Both of these traditional approaches are costly and time-consuming. In addition, the data and information obtained by these methods is rather limited and does not always yield all the designers' requirements.

In *principle*, CFD models are capable of providing, both heat transfer data required by thermal models and the detailed information necessary to assess environmental performance. The interrelationship between the dynamic thermal models and microclimate models is illustrated by the schematic diagram shown in Figure 1. The link between the two models is shown by shaded arrows and the iterative process of updating convective heat transfer data in thermal model and boundary conditions in CFD model is represented in Figure 1 by dashed lines.

In *practice*, CFD models have a number of limitations (see section 3), and are very costly in terms of computing resources. The author and his co-workers have argued (see, for example, (4)) that 'intermediate-level' models offer the best prospect of meeting the needs of dynamics thermal models, in terms of economy and user-friendliness for providing convective heat transfer data. Therefore, CFD models should be used as an independent tool for environment thermal comfort and safety assessment, rather than being integrated into the thermal models.

3 COMPUTATIONAL FLUID DYNAMICS MODELS

3.1 Background

All thermo-fluid problems are governed by the principles of conservation of mass, momentum, thermal energy and chemical species. These 'conservation laws' may each be expressed in terms of partial differential equations, the solution of which provides the basis for the computational fluid dynamics (CFD) model. CFD models solve, numerically, the governing conservation equations in order to generate field values for the velocity components, the static pressure, the temperature and concentration of chemical species. The

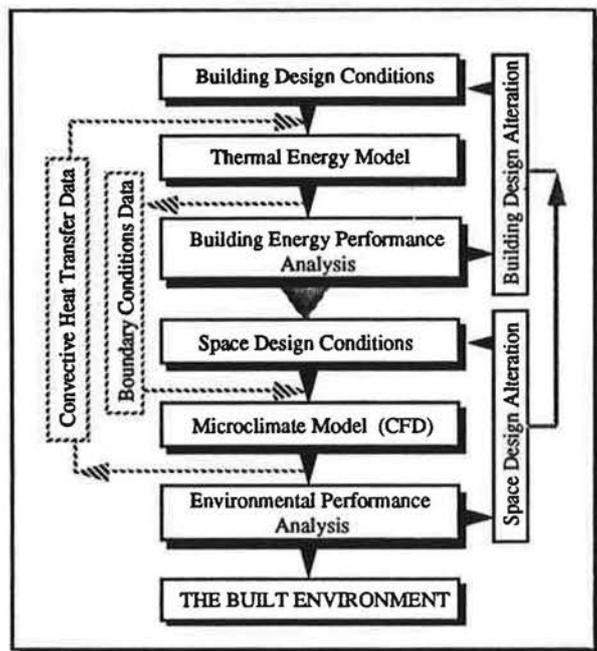


Fig 1 Interrelationship between the thermal energy and the microclimate models

governing equations for air flow, thermal field and concentration species may be represented by a common form, using tensor notation (6):

$$\frac{\partial (\rho\phi)}{\partial t} + \frac{\partial (\rho u_j \phi)}{\partial x_j} = \frac{\partial \{ \Gamma_\phi (\partial\phi/\partial x_j) \}}{\partial x_j} + S_\phi \quad (1)$$

where u_j are the time-averaged velocity components in the coordinate direction x_j , ϕ are any of the dependent variables, Γ_ϕ are the effective diffusion coefficients, S_ϕ are the sources or sinks, ρ is the fluid density, and t is time.

These governing flow equations are strongly inter-linked with no obvious equation available for the static pressure that appears in the momentum equations. Therefore, it is necessary to use numerical solution techniques for their solution. The numerical solution of the governing flow equations requires some discretization of the flow domain into a finite set of elemental or control volumes, formed by computational grid (2) and (6). The differential equations may then be integrated over each elemental volume of the computational grid. This leads to a set of algebraic equations in the following finite-volume form:

$$(a_p - S'_p) \phi_p = \sum_n a_n \phi_n + S_p \quad (2)$$

$$a_n = D_n \alpha (|Pe_n|) + [|0, \pm C_n|]$$

$$a_p = \sum_n a_n$$

where, indices p and n denote the central computational grid point and its neighbouring points respectively, C and D indicate the strength of the convection and diffusion respectively, $\alpha (|Pe_n|)$ is a weighting function, and the symbol $[|a,b|]$ denotes the greater of a and b . The source term S_ϕ in Equation 1 is evaluated using a linearised expression $(S_p + S'_p \phi_p)$ in order to enhance numerical stability.

These algebraic equations are then solved in a finite-volume CFD model by an iterative manner (see Figure 2). The iterative solution continues until the imbalance or error in the equations is sufficiently small to be considered negligible.

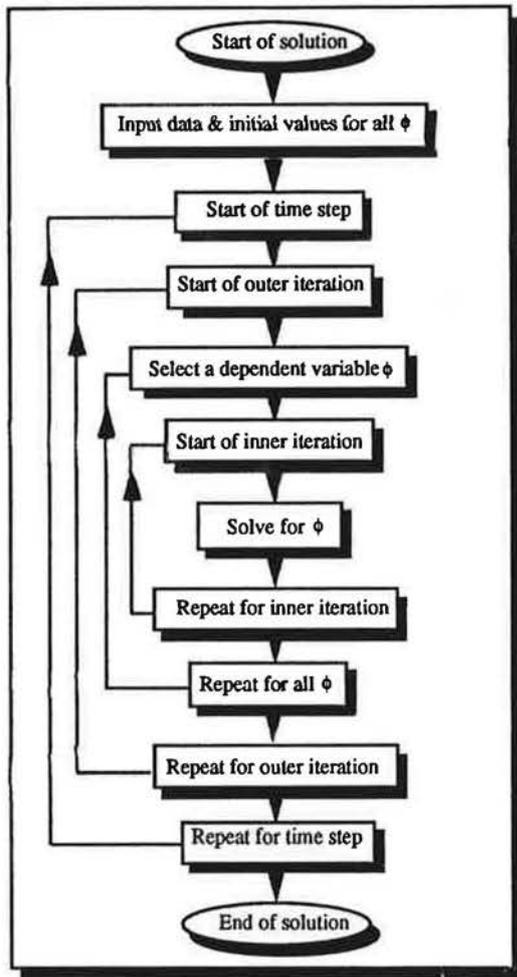


Fig 2 Iterative solution sequence

3.2 Capabilities

Today, CFD codes have grown much in complexity, taking advantage of the speed and power of new computers, and can offer a powerful and versatile computer-aided-engineering design tool. In the most general form these codes are potentially capable of handling time-dependent, turbulent, chemically reacting, compressible, non-Newtonian, multi-phase flows in complex geometries. Heat exchange by means of convection, conduction and radiation in both fluid and solid and the effect of thermal buoyancy and gravitational forces can be studied.

The commonality of the thermo-fluid processes in application areas, and the form of the governing equations, allow the same CFD code to be used in a number of engineering practical situations, for example:

- External aerodynamics of aircraft, motor cars, ships
- Heat transfer and combustion processes within internal-combustion or gas-turbine engines
- Thermal-hydraulics of nuclear reactors, steam generators, condensers, etc.

In the context of the built environment, CFD models may be used as an efficient and powerful tool for:

- *Air movement and thermal comfort assessment*
This is an important aspect of air conditioning performance analysis and preventing problems, such as 'sick building syndrome', which are mainly associated with poor air movement and temperature distribution within the space.
- *Smoke and other pollutants movement analysis*
The effectiveness and performance of the ventilation system in removing the smoke as a result of fire or other contaminants is important in the safe design of buildings.
- *Convective heat exchange calculation*
The accuracy in the thermal energy performance analysis of buildings is limited by uncertainties in data, particularly for convective heat transfer rates (see Section 2).

In addition to the above, CFD may be used to predict thermo-fluid phenomena in the natural environment, such as:

- *Pollution analysis*
The spread of smoke and other pollutants discharged from chimney or chemical plant into the atmosphere, the dispersion of sewage in the ocean, etc.
- *Climatic analysis*
The prediction of atmospheric gravity-influenced turbulent flows, analysis of microclimate effects on humans, etc.

Those CFD codes that could be used in all of the above application areas and more are categorised as 'general purpose' CFD programs. Most of these codes are notoriously difficult to use. However, in the last few years, the advances in computer graphics have enhanced the user-friendliness of most of these codes. Furthermore, a range of 'special-purpose' CFD codes have been developed and optimized for particular application areas.

3.3 Applications in the Built Environment

Computational fluid dynamics models, have a wide range of application areas in buildings, some of which are given below:

- *Atria*
Atria with large glazing have gained popularity within the new architectural design of office complexes. CFD can be used to analyse the environmental performance under various summer and winter climatic conditions for over-heating and cold down-draughts respectively.
- *Art galleries and museums*
Poor air movement, temperature and humidity distribution in art galleries and museums may damage paintings and other expensive displays. Therefore, CFD simulation has a high potential in design and maintenance of these environments.
- *Shopping centres, Tunnels, Airport terminals, etc.*
In addition to analysis of heating, cooling and ventilation of these spaces. CFD simulation can be used as a powerful tool to predict the smoke movement and spread of fire. In recent years, this exercise has taken a high profile in the design and control of safe public building enclosures.

- **Air conditioned offices.**
CFD is a useful tool in predicting the flow pattern and temperature distribution within mechanically- or naturally-ventilated rooms. The performance and position of the air supply and exhaust diffusers, or radiators, etc. can be optimized.
- **Clean rooms and Operating theatres.**
In the design of tightly controlled environments, CFD simulation may be used to predict the flow pattern and contaminant movement.
- **Industrial buildings.**
CFD simulation may be used to predict the performance of the ventilation and air distribution system within industrial buildings. The simulation could include the heat distributed from machinery, the movement of flying dust, etc.

3.4 Modelling Requirements & Limitations

Geometrical aspects

The first step in the solution of Equations (2) is the discretization of the flow domain, and the definition of the points at which variables are located. Discretization of the flow domain must conform to the boundaries in such a way that boundary conditions can be accurately represented and allow the computational cells to be small in regions with steep property gradients, such as near the walls, around obstacles, regions with high curvature, etc. Domain discretization is provided by a computational grid, generated using an appropriate coordinate system. Most building spaces may be discretized by using rectangular cells (or elemental-volumes) and adopting simple Cartesian coordinate system. However, some difficulties may arise in specifying angled or curved surfaces, which have to be represented by 'best step-wise' fit to a grid and blocking off cells (see, for example, Figure 3). The CFD models using this approach are very efficient in running time, but the accuracy of the solution may be affected.

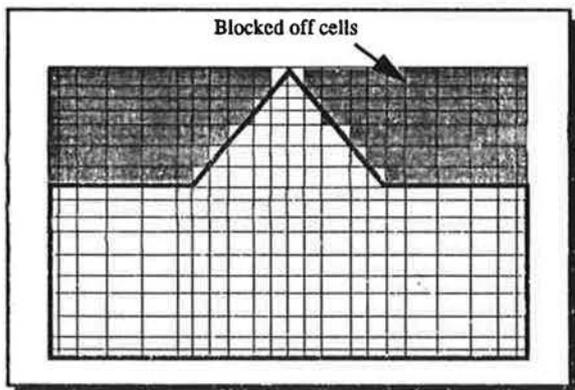


Fig 3 Non-uniform Cartesian grid

The numerical grid generated techniques, using the boundary-conforming (body-fitted) coordinate system may be used to generate a grid to fit irregular boundaries. This enhances the accuracy of the solutions for non-rectangular geometries. Some CFD codes use only a 'simply-connected' regions grid generator, in which they can handle spaces without any obstacles inside them (Figure 4). These models require a blocking off capability, in order to include objects inside the domain. A weakness in these models is that the objects will be represented with best fit grid accuracy. Those CFD models with 'multiply-connected' regions grid generators could include obstacles, but may become complicated to use when there are many objects.

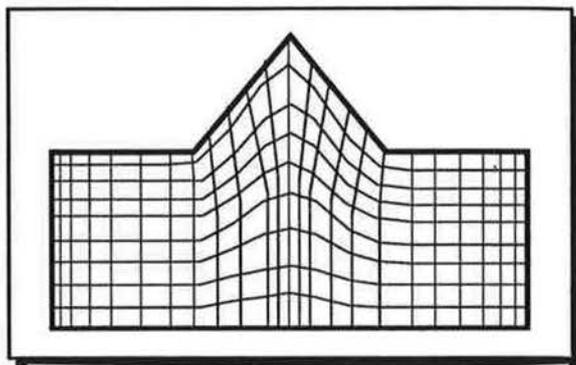


Fig 4 'Simply-connected' body-fitted grid

The new generation of 'composite' grids consider the flow domain to be divided into sub-domains (sub-regions), bounded by generally curved sides, and within each sub-domain an individual coordinate system being generated. The overall coordinate system, covering the entire domain, is then formed by joining the sub-domains at the sub-region boundaries (7).

The accuracy of the solution obtained by CFD simulation usually relies heavily upon the degree to which the solution depends on the grid arrangement. Therefore, in all CFD simulations a grid independence test must be sought by increasing the number of the grid lines, or concentrating them into regions where large variations in the variables occur, such that no significant change is observed with further increase. In most building applications, it is therefore desirable to adopt a flexible three-dimensional body-fitted grid generation with local grid refinement capability. Local grid refinement allows the key areas of the flow domain and its boundaries, such as inlets, heat sources, etc. to modelled more accurately and economically (Figure 5). However, such models could seem more difficult to use when compared with those using simple Cartesian coordinates.

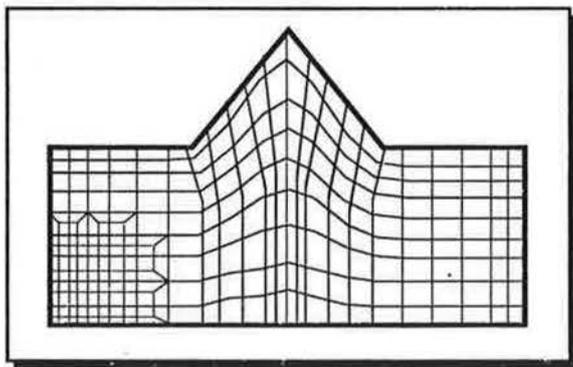


Fig 5 Body-fitted grid with local grid refinement

Boundary Conditions

In building applications, the solution domain is usually bounded by solid surfaces (such as walls, floor, ceiling or roof, doors and windows) and fluid surfaces (such as air supply and exhaust registers). Because of the 'elliptic' nature of the flow in the built environment, the condition at any point in the flow can be influenced by other points. Therefore, it is necessary to supply boundary conditions for all variables at all boundaries of the flow domain. These boundaries could be a specified value of variable or value of the associated flux, or a relation between the variable and the flux.

The time-dependent interaction between the external conditions, building structure fabric and internal conditions, means that the domain boundary conditions vary with time. Therefore, it is desirable to link a CFD model with a dynamic thermal model (see Figure 1). However, since CFD models require a sophisticated iterative solution procedure (see Figure 2) on very small time scale (ie. seconds rather than the hours that are usually used by thermal models), this link could increase the computer execution time dramatically (8). Some compromises may be made on the scale of interaction, for example, performing steady-state CFD simulation for every few hours of thermal model simulation and using the results of previous CFD simulation for the initialization of the domain.

Time-dependent flow simulations usually require substantial computing resources, therefore, in practice, boundary conditions may be assumed to be steady-state, based on the analytical or experimental results, except when CFD is used to predict the dispersion time of gases or smoke; for example, in evacuation time analysis.

In turbulent flows, viscous and turbulent stresses are of the same order of magnitude near the wall. This forces the values of turbulent transport properties to fall to their laminar values and the result is a steep, non-linear variation with distance from the wall in dependent variables and their gradients. Most CFD models use the so-called 'wall-functions' in order to bridge the steep property gradients close to the solid surfaces (9). These are based on the bilogarithmic behaviour of the mean velocity and temperature near solid walls. The present generation of wall-functions are not appropriate for recirculating flows and will give rise to error in, for example, heat transfer calculations (10).

Flow Type

The transient radiation, conduction and convection heat transfer processes in and around buildings gives rise to very complex fluid flow problems. The airflow around buildings are usually turbulent flows, while the Reynolds numbers (the ratio of inertia to viscous forces) for most flows within the built environment are in the transition range. Even in the turbulent regime, there is currently no universal turbulent model available that can reflect the behaviour of the full range of complex turbulent flows observed in buildings (11).

In turbulent flows, the closure of the governing equations (Equation 1), may be achieved by using a 'turbulence model'. The most commonly used turbulence model is the $k-\epsilon$ model, which involves the solution of two additional partial differential equations for the turbulence kinetic energy (k) and its dissipation rate (ϵ). Other models such as Reynolds stress and large-eddy simulation models (12-14) may be used to achieve greater accuracy (depending on the application), but they increase complexity and require more computing resources.

Buoyancy effects are common in the built environment, and should be incorporated into discretization equations. In most building applications, air density can be assumed constant throughout the flow domain. Therefore, buoyancy effects may be introduced into the solution by the adoption of the so-called Boussinesq approximation (see for example (2)). However, this usually reduces the rate of convergence.

Solution and Controls

The solution method shown in Figure 2, is aimed at solving a set of nonlinear, interlinked equations in an iterative, 'point-by-point' or 'line-by-line' manner. In this method, it is necessary to examine how the current solution approximates to the exact solution of Equation 2 at the end of each iteration, for each variable. Therefore, convergence criteria may be defined, for example, to be based on the imbalance source for Equation 2.

The iterative solution should, in principle, handle any non-linear and interlinked equations. However, the use of some form of under-relaxation is found to be very useful, with 'cell-by-cell' or 'line-by-line' iterative solution methods. It reduces the magnitude of current error level in the field, while preventing the divergence in the iterative solution of the equations. There are several ways of introducing under-relaxation, for example, 'linear' approaches via relaxation factors and 'inertia' methods, by introducing inertia terms into the discretized equations. However, there are no general rules for describing the optimum values of relaxation factor and inertia term. Suitable under-relaxation factors or terms can be found by experience and from exploratory computations for given problems.

The accuracy of the solution obtained by CFD simulation usually depends on the degree to which the solution satisfies the discretized equations. This can normally be assessed by the level of imbalanced error-sources within discretized equations. A graphical representation of these sources gives a useful indication on convergence, for example Figures 6 and 7 show the solution is converging, while Figures 8 and 9 show the solution is diverging and oscillating respectively.

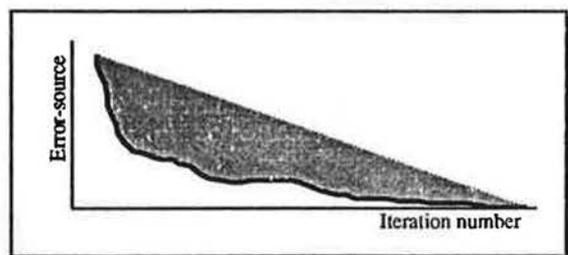


Fig 6 Converging solution

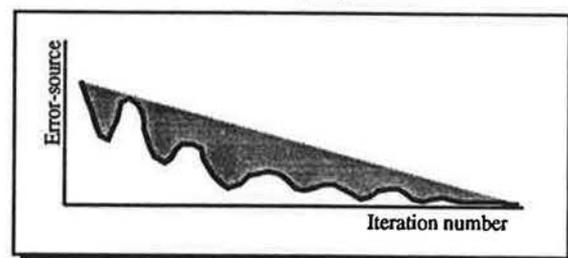


Fig 7 Converging solution

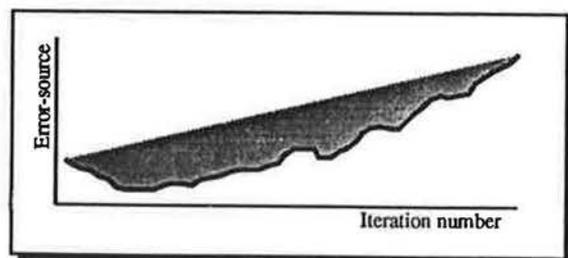


Fig 8 Diverging solution

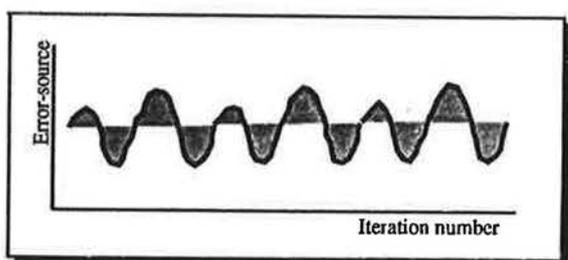


Fig 9 Oscillating Solution

Results

The data obtained from a CFD simulation could include the values of all dependent variables, such as air velocity, temperature distribution, pressure distribution, concentration of chemical species, etc. for each computational control-volume. This quantitative data is usually sufficient for the safety assessment of the environment. However, the measure of thermal comfort by the use of air velocity and temperature only, can sometimes be misleading and it is desirable to calculate the resultant temperatures, in contrast to dry air temperatures commonly calculated in general-purpose CFD models. The resultant temperature index recommended for use in the UK requires information about air velocity and temperature, and mean radiant temperature (15). The mean radiant temperature at a grid point within the domain is a function of the surface areas, shapes, surface temperatures and emissivities of the enclosing elements seen from that point. The calculation of the mean radiant temperature may involve additional complex ray tracing techniques for determining the shape factors for all surface elements viewed from each grid point.

The advances in computer graphics have allowed the development of graphical display tools, which can be used for viewing the correctness and resolution of the generated grid, monitoring the convergence and displaying the results. Most CFD software incorporates an interactive graphics program, capable of displaying field velocity vectors, temperature, pressure and concentration contours, etc. in two- and three-dimensional domains (see for example Figures 10). However, due mainly to hardware portability issues, the functionality of the graphics utilities within commercially available CFD codes are currently limited.

The basic requirements for a CFD visualization utility for the generation, analysis and presentation of results are:

- Full three-dimensional capability
- Rotation, zoom and pan facilities
- Multiple viewing management
- Vector and contour plotting
- Streamline particle tracking capabilities
- Cursor pointing display data facility
- Text annotation and editing

Userfriendliness

CFD models have been mainly used by academics, specialist consultants or research and development departments in large companies, and particularly in specific application areas, such as in the aerospace, automotive, chemical and process, and nuclear industries. The reason for this is the complexity in use and costs of these models, rather than the lack of need in other sectors. The building industry in particular found CFD software more difficult to use compared with more familiar computer packages; for example, thermal energy calculation codes.

The environmental and building designers' interests are only in the result (mainly graphical) of CFD simulation, rather than the processes involved in obtaining the results. In the last few years advances in computer graphics allowed the development of graphical user interface for most engineering software, including some of the CFD codes. User interface technology, potentially, should allow designers to access to the power of CFD, with little or no knowledge of the CFD mathematical modelling techniques. This means a CFD graphical interface must provide a comprehensive collection of user-interaction functionalities which typically involve from setting up the initial geometrical data, through simulation, to the actual interrogation of the results in such a way that the user is able to extract the information that is re-

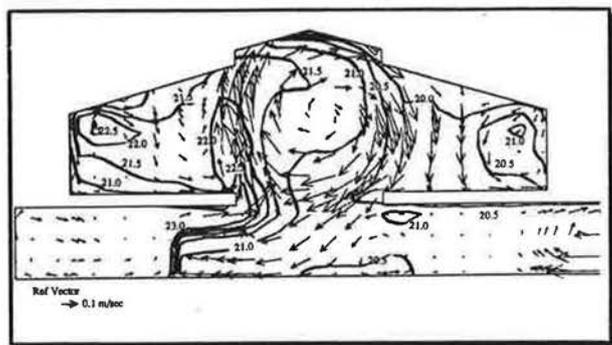


Fig 10 Predicted air velocities and temperature distribution in an open atrium office building

quired. This may be achieved by dividing the main process of solving a complete flow problem into three basic units or processors, linked together via an intelligent user interface environment. Figure 11 illustrates the basic functionality of these processors.

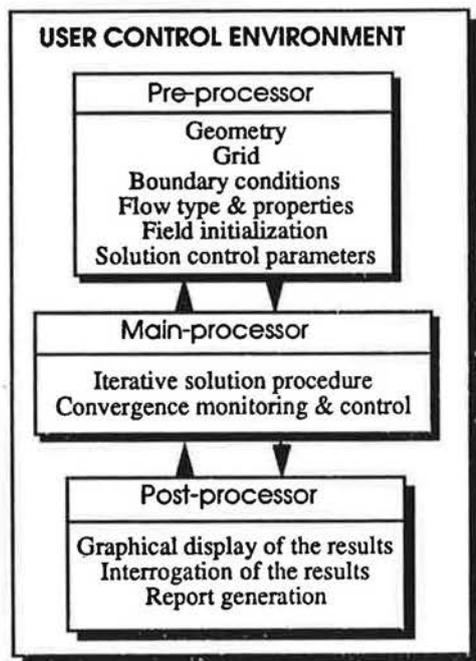


Fig 11 User interface control environment

Resources and Costs

Microclimate designs of buildings are complex, time consuming and usually require considerable resources and expertise in the field of building physics and fluid dynamics for obtaining meaningful results and analysing them.

The execution time is dependent upon the problem under consideration, the accuracy required and the computer used, for example:

- Domain dimensionality**
In most buildings the assumption of two-dimensional flow situations is not valid and complete three-dimensional studies must be carried out. This increases the execution time dramatically.
- Domain representation**
In order for a computer model to be able to represent the flow domain realistically, it should include all internal and boundary features that may affect the flow pattern, therefore

usually a large number of computational grid lines are required, which increases the run time.

- **Nature of the flow**
Steady-state simulations are often sufficient for thermal comfort and safety analysis, but there are situations where, physically, this assumption is not valid and constraining the solution to steady-state may result in divergence in the CFD iterative solution. Therefore, a time-dependent solution should be performed which requires much higher computer time.
- **Computer hardware**
The execution time is highly dependent upon the performance of the computer hardware. In most three-dimensional building spaces, the transient simulation requires a run time in the order of days or even weeks on a typical workstation computer. However, the same simulation may be executed on a high performance vector machine in a matter of hours.

Today, most commercially available CFD codes are available on a variety of computer systems: PCs, workstations, minicomputers, mainframes and vector super computers. The licence fee usually depends on the capability of the software, computer power and the duration of the licence. For example, a one year licence for PCs (368 and 486) could be around £4000-8000 and for workstation computers around £5000-20000, depending on the power and performance of the computer hardware.

4. CONCLUSION

A controlled and safe building environment can be designed, by detailed analysis of microclimate performance of the building, using advanced CFD computer simulation techniques. CFD models are capable of simulating the complex fluid flow and heat transfer problems common in the context of the built environment. However, they require far greater computer time, compared with simpler calculation methods. This has prohibited their direct use in providing heat transfer input data for dynamic building thermal models. Indeed the author and his co-workers have previously shown (4) that their simpler convection models are more appropriate for this purpose. CFD models, therefore, should be used where accurate prediction of field air velocity, temperature distribution and concentration of species is required, for thermal comfort and safety assessment of the environment.

The complex nature of the governing flow equations, associated turbulence models and numerical solution procedures, have made CFD codes far more difficult to use than the architectural and building services software tools. The new generation of CFD software with enhanced intelligent graphical user interfaces should, potentially, reduce the level of the complexity in use and expertise required in computational fluid dynamics modelling. However, the expertise and the understanding of the thermo-physics and thermo-fluid in buildings, for the analysis and appropriateness of the results, is always essential in any thermal and microclimate building modelling.

In addition to computer and expertise resources, CFD software currently has a number of limitations in mathematical modelling:

- **Turbulence closure**
There is currently no universal model available that accurately deals with the full range of turbulent and transitional flows observed in the context of the built environment

- **Wall functions**
The algebraic wall functions used in most CFD software are not appropriate for recirculating flows and may give errors in, for example, heat transfer calculations. The alternative approach of low Reynolds number modelling down to the wall is not economically feasible because of the large number of grid points that would be required for building flows.
- **Buoyancy effects**
Applications with strong buoyancy-driven flows usually require a large number of iterations and are very slow in convergence.
- **User environment**
In most CFD codes, the user interfaces (if any), geometry generations (if any) and grid generation methods are poor.

Nevertheless, CFD simulations could enable the environmental and building designers to:

- **Generate new design concepts**
- **Analyse the performance of their design**
- **Perform design confirmation prior to commitment of major investment.**

These may bring about a wholesale reappraisal of the design of environmentally conscious buildings, more quickly and economically, compared with alternative microclimate prediction methods.

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