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CAFE - A COMPUTER PROGRAM TO CALCULATE THE FLOW ENVIRONMENT.

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The program CAFE has been prepared for application to engineering problems involving fluid flow and heat transfer. Based on a finite-difference method, its main advantage over other programs is its generality, which enables problems requiring a variety of different boundary conditions to be studied. A description is given of the mathematical formulation of the program, its major features and several examples of its application for the study of internal and external flows. The predictions of the program appear qualitatively reasonable and can be up to an order of magnitude cheaper than corresponding experimental studies.

INTRODUCTION

Research into the mathematical modelling of industrial processes involving fluid flow and heat transfer has advanced to such an extent over recent years that many computer programs have been developed for specific applications. However, the ultimate goal of universal applicability, high precision, cheapness and ease of use of such programs is still remote. Over the past few years, the authors have been engaged in the development of a suite of computer programs under the generic name CAFE (Computational Atkins Flow Evaluation) which can be used on behalf of clients to study fluid flow either within or around buildings or industrial equipment, taking into account the effects of heat transfer.

The purpose of the present paper is to describe the current status of these programs, to indicate their range of applicability and to describe the future developments which are envisaged. Several examples of the application of the CAFE suite are given, including the solution of the following flow problems:

(a) Ventilation of a building to reduce concentrations of dangerous gases;

(b) Discharge of an effluent in an estuary;

(c) Transport of particles in a duct;

(d) Dispersion of hot exhaust gases from turbo-generators on an offshore platform.

The mathematical description of the flow phenomena is considered first. The governing differential equations and some of the auxiliary algebraic equations are also described. Then the numerical procedure for the solution of the differential and algebraic equations is briefly presented. Some of the user-oriented features of the program are described, together with an indication of the developments which are currently being undertaken.

For simplicity of discussion, only two dimensional situations are considered in the present paper. However, the extension to three dimensions is straight forward (Moult, 1978).

The terms involving the velocity divergence div v in the source terms of the momentum equations have been ignored. For constant density flows div v is identically zero. For most other flows handled by the present procedure, div v is expected to be small compared to other terms and is omitted for simplicity.

For turbulent flows, the viscosity μ and the Prandtl or Schmidt numbers, σ, appearing in the table must be replaced by their effective values μ_{eff} and $\sigma_{eff,\phi}$.

The turbulence model

The turbulence model incorporated in the present procedure is the high Reynolds number (k,ε) two-equation model of Harlow and Nakayama (1968) as modelled by Launder and Spalding (1974). This model requires the solution of two differential equations, for two turbulence characteristics, the kinetic energy of turbulence k, amd its dissipation rate, ε.

The governing differential equations are presented in the Table, where G_k is the generation terms for the kinetic energy of turbulence and is given by

$$G_k = 2\mu_T \left\{ \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 \right\} \tag{2}$$

In this model the turbulent viscosity, μ_T, is related to k and ε via

$$\mu_T = C_D \rho k^2/\varepsilon \tag{3}$$

and the effective viscosity is given by

$$\mu_{eff} = \mu_T + \mu_L \tag{4}$$

The local effective exchange coefficient, $\Gamma_{eff,\phi}$ for the transport of the scalar property ϕ, is calculated from

$$\Gamma_{eff,\phi} = \frac{\mu_L}{\sigma_{L,\phi}} + \frac{\mu_T}{\sigma_{T,\phi}} = \frac{\mu_{eff}}{\sigma_{eff,\phi}} \tag{5}$$

where μ_L and $\sigma_{L,\phi}$ are the molecular viscosity and the laminar Prandtl or Schmidt number, respectively, and μ_T and $\sigma_{T,\phi}$ are their turbulent counterparts, to take account of the effect of turbulence on mixing. This turbulence model includes four constants, their recommended values being: $C_D = 0.09$, $C_1 = 1.43$, $C_2 = 1.92$, $\sigma_{k,eff} = 0.9$. The value of $\sigma_{\varepsilon,eff}$ is calculated from the relation $\kappa^2/(C_2-C_1)C_D^{\frac{1}{2}}$, where κ is the Von Karman constant (= 0.4).

THE NUMERICAL SOLUTION PROCEDURE

The governing equations (1) are solved numerically subject to the appropriate initial and boundary conditions. The grid layout used is the 'staggered' grid system suggested by Patankar and Spalding (1972) for parabolic flows. It is formed by planes running parallel to the coordinate axes. Where the two sets of plane intersect are the 'main nodes' at which all flow properties, except velocities, are evaluated. The velocities are stored at locations 'staggered' with respect to the main nodes, in the corresponding direction, as shown in Figure 1. Finite-difference equations for a grid node are obtained by integrating the differential equations over a control volume surrounding the grid node. For this integration, information on the variation of the flow properties between two neighbouring nodes is needed. The diffusion fluxes through a control-volume face are evaluated by assuming a linear variation of the flow properties in the direction normal to the face. The evaluation of the convection fluxes through a control-volume face is performed using the upwind value of the convected property (Gosman et al, 1969). The above integration yields a five-node finite-difference relation at each node, P, of the form:

where ϕ_{given} is the value to the property in the solid. Substitution of these expressions into equation (6) results in the value of the property ϕ at the point P being fixed as ϕ_{given}.

(iii) Next to a wall or obstacle the boundary of the flow domain cuts the links joining a node P to its neighbours. The nodes that lie outside the boundary have no real significance and are modified so that they do not influence the node under consideration. This modification involves setting the neighbour node coefficient (either A_x^+, A_x^-, A_y^+ or A_y^-) to zero. In addition, the presence of a boundary brings in influences like shear stresses, heat fluxes, etc. These effects must be expressed as additional source terms for the control volume that is affected.

(iv) and (v) Mass and momentum sources are treated by modifying the appropriate source terms in equation (6), so that they become

$$Su^{(new)} = Su^{(old)} + m * \phi_{inj}$$
$$SP^{(new)} = SP^{(old)} - m \qquad (7)$$

where 'm' is the mass source and ϕ_{inj} is the value of the property injected into the control volume. In the case of a source of mass but not momentum then ϕ_{inj} is zero.

(b) Presentation of the results

Whenever possible, the policy is to provide pictorial output rather than lengthy tables of numbers. Typically plots of temperature contours, streamlines and velocity vectors are obtained, which enable rapid dissemination of results and comparison with the predictions of other methods.

APPLICATIONS

(a) A ventilation problem

The geometry of the problem analysed is shown in Figure 2, and consists of a stack of warm coal (KLM) enclosed in a building AEJ. Methane is given off from the surface of the coal stack and disperses in the building. There are two inlets, AB and NJ, to the building through which outside air is entrained, and two outlets (CD and FG) from which the mixture of air and methane escapes.

The problem is to determine the steady state concentration of methane in the building, bearing in mind that when a concentration of greater than 5% occurs then explosions are possible.

The two equations for u and v, the continuity equation, the equations for k and ϵ, the enthalpy equation and an equation for the mass concentration of methane, m_{meth}, in the building are solved.

The problem was solved using a non-uniform 36 x 19 grid with the greater number of grid lines being laid in the x-direction. 150 iterations were required to reach a converged solution.

Results. Figures 2 (a) and (b) show the velocity vectors and methane concentration contours predicted by the solution procedure. The velocity field consists of two closed circuits, one on each side of the coal stack. The methane is distributed in layers, without the presence of any potentially dangerous pockets of methane.

(b) An effluent problem

Figure 3 shows a plan view of the sea in the region of a coastal power station. The problem is to calculate the temperature distribution in the neighbourhood of the power station outfall resulting from the warm water discharge. Equations are solved for u, v, pressure correction, k, ϵ and temperature T. A non-uniform equations are solved in this model, one for the fuel mass fraction, m_{fu}, and the other for the composite mass fraction, f, defined to be

$$f = m_{fu} - m_{ox}/S \tag{9}$$

where m_{ox} is the mass fraction of oxygen.

Expressions for the rate of generation of fuel by chemical reaction can be found in the literature, e.g. Spalding (1976). An equation of the form of (6) can thus be derived, provided that the assumption is made that the exchange coefficients of fuel and oxidant in the equation for f are equal at each point in the flow. The inclusion of chemical reaction means that the stagnation enthalpy h needs to be redefined as

$$h \equiv h_o + \tfrac{1}{2}\,(u^2 + v^2) \tag{10}$$

where h_o is the specific enthalpy, given by:

$$h_o = C_p T + m_{fu}\, H_{fu} \tag{11}$$

where H_{fu} is the heat of combustion and C_p is the specific heat at constant pressure.

(b) The radiation model

The model which is to be incorporated into the program is of the four-flux variety deriving from the works of Schuster (1905) and Hamaker (1947). This model accounts for the effects of radiation by reference to the four fluxes I, J, K and L in the positive and negative x and y directions. (Note that in three dimensions a six-flux model can be similarly defined.)

(c) Two-phase flows

A two-phase flow algorithm is being developed which will allow flows to be studied in which the phases move with unequal velocities. The technique is based on the solution of two sets of momentum equations, one for the liquid and the other for the vapour. The continuity equation is replaced by an equation relating the mass fractions of liquid and vapour.

CONCLUSIONS

The examples given in the paper indicate that a general purpose computer program can be developed for the study of a wide range of problems involving fluid flow and heat transfer. Although the examples given have all been two-dimensional, three-dimensional situations have also been studied successfully. The developments to the program currently being undertaken will considerably extend its possible applications. However, these developments will be made within the frame work of the original program specification, namely that the program should be user-oriented, i.e. simple to modify for a variety of different boundaries and yield solutions in forms that are easily assimilated.

Although the predictions of the program have been verified for simple test problems such as pipe and jet flows for which experimental measurements exist, there is a need for detailed full-scale measurements with which the programs can be compared. In this way the various constants appearing in the governing equations can be more finely tuned.

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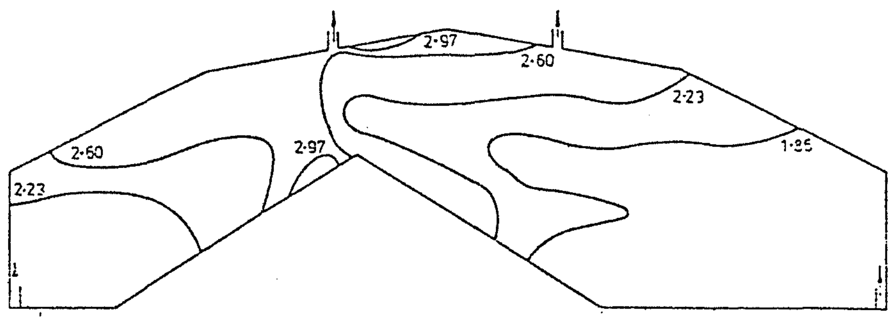

Fig. 2(b) Concentration of methane %

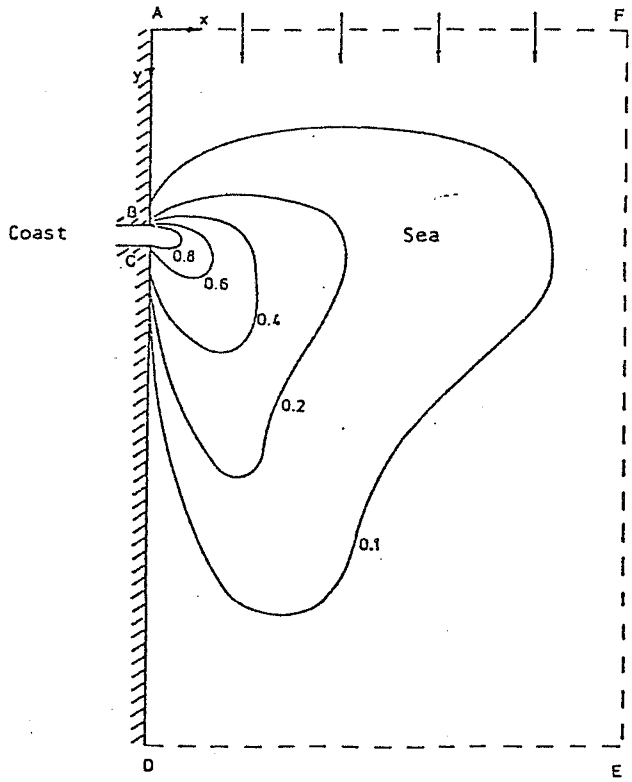

Fig. 3 Temperature contours (% of outlet value)

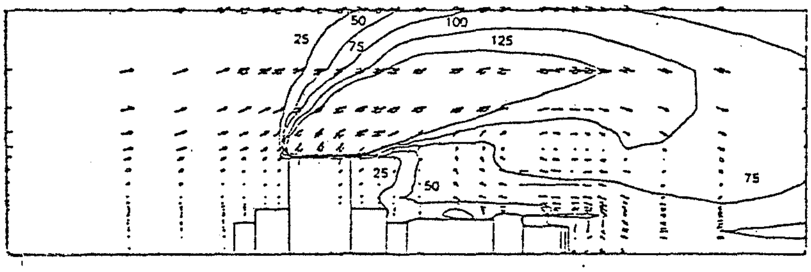

Fig. 6 Velocity vectors and temperature contours