Chapter 2

Compressible computer code

2.1 The numerical scheme

In the present analysis a two-step explicit and time-marching finite difference scheme is adopted to express the partial differential equations for the compressible flow. The finite difference formulations are given in Appendix A. However, some essential features of the numerical method are discussed here.

To analyze a two dimensional flow of an ideal gas, four dependant variables: two velocity components and any two other thermodynamic properties are required. For the compressible flow approach, the energy equation is coupled to the momentum and continuity equations, and there are four coupled differential equations to work with. When these differential equations are rearranged in a conservative form, they can be cast in a 'vector' form equation in the form:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0 \quad (2.1)$$

where the vectors $\mathbf{W}$, $\mathbf{F}$, and $\mathbf{G}$ are ordered sets of the variables ρ , ρu , ρv and ρe . Physically, $\mathbf{W}$ represents the quantity that may accumulate in the control volume, $\mathbf{F}$ the flux of $\mathbf{W}$ in the x direction, and $\mathbf{G}$ the flux of $\mathbf{W}$ in the y direction. For the inviscid case, neglecting the body forces, the Euler equations are obtained, and the matrices $\mathbf{W}$, $\mathbf{F}$ and $\mathbf{G}$ become:

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Numerical Simulation of Ventilation Air Movement in Offices

by

A. Alexios Soultogiannis

Dipl. (Mechanical Engineering), Aristotle U. of Thessaloniki

**A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfilment of
the requirements for the degree of
Master of Engineering**

**Department of Mechanical
and Aerospace Engineering
Carleton University
Ottawa, Ontario
November 1990**

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submitted by
A. Alexios Soultogiannis, Dipl. Eng.,

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Abstract

The present thesis presents simulation models for the prediction of the air movement in ventilated spaces, and more specifically in workstations in an office complex. The nonlinear differential equations that describe the air motion are solved by using finite difference methods.

Based on two different approaches, two models were developed: the first one considers the flow as compressible, while the second one as incompressible. A comparison of the numerical results obtained by the incompressible model with experimental data, shows that the general trend of the airflow is reproduced to satisfactory tolerance. Contrary to the incompressible approach, the numerical predictions of the compressible model are in significant deviation from the experimental values. Consequently, it is recommended that the incompressible model should be preferred for further development.

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Nomenclature

A	Area
Ar	Archimedes number
Ar_c	Corrected Archimedes number, defined as $\frac{0.62}{D} Ar$
a_i	Coefficient of finite difference equation for the INCOMP code
B	Area of the diffuser outlet
B₁	Distance from bottom of inlet to bottom wall
B₂	Distance from bottom of outlet to bottom wall
C	Gas concentration
c	Local speed of sound
C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
d₁	Width of the inlet opening
d₂	Width of the outlet opening
d₃	Distance from left side of partition to the wall or partition at the left
d₄	Distance from right side of partition to the wall or partition at the right
D	Characteristic dimension of a room, as defined by Zhang et al. [5]
e	Total energy per unit mass
F_i	Diffusive damping coefficient for i direction
H	Height of room
h₁	Height of partition
h₂	Distance from bottom of partition to the floor
k	Kinematic energy of turbulence
L	Length of room
m	Mass flow rate
P	Pressure
R	Gas constant

Re	Reynolds number, defined as $\frac{U_i d_i}{\nu}$
T	Temperature
t	Time
t_1	Thickness of partition
U_i	Diffuser air velocity
u	Velocity component in x direction
v	Velocity component in y direction
x	Longitudinal coordinate
y	Vertical coordinate
z	Lateral coordinate
γ	Ratio of specific heats
ϵ	Turbulence energy dissipation rate
μ_t	Turbulent or eddy viscosity
ρ	Density of the fluid
ν	Kinematic viscosity of the fluid

Chapter 1

Introduction

1.1 Objectives and outline of the thesis

The objective of this research is to develop an appropriate computer model for the simulation of the ventilation air flow in an office complex. The major aim of ventilating spaces is to distribute heat and fresh air, to control moisture and to remove contaminants. The understanding of the air movement induced by ventilation becomes extremely important in fundamental studies of building thermal analysis, indoor air quality, and thermal comfort. Therefore a designer of ventilated rooms is required to know the flow characteristics of a given ventilation arrangement for a particular room geometry, prior to the installation of the ventilation system.

The air movement in ventilated spaces can be described by a set of conservation equations: the continuity, momentum, energy and component conservation equations. Unfortunately, no exact solution to these coupled nonlinear differential equations is available, and proposed empirical equations present dimensional uncertainties even for simple forms of jets [1]. Predictions are often obtained by setting up the flow configuration in a model or a full scale room. Flow visualization and measurements are used to get a picture of the flow, but such investigations are expensive, and it can be difficult to alter the geometry and the inlet conditions, especially for a full scale room. Moreover, the validity of the model tests is still questionable [1]. Consequently, a good alternative is to use numerical techniques

to investigate the air flow pattern.

For this purpose, two different computer codes were developed by the author, based on fundamentally different approaches: The first one, the COMP code, solves for the compressible unsteady state, while the second one, the INCOMP code, for the incompressible steady state. However, the COMP and INCOMP codes share some common assumptions, which will be discussed briefly.

A two dimensional approach is adopted for both codes as a preliminary treatment of the flow regime in a ventilation system. Since the solution is two dimensional, unit depth is assumed in all computations. This assumption is valid only in connection with the size and location of diffusers in a room. If the inlet and outlet slot diffusers are located at the center of the room, and the openings are not much shorter than the width of the room, then the resulting flow field is practically two dimensional [2, 3]. Both codes assume no contamination sources, solving only for the air velocity field. The air temperature field is assumed to be uniform and isothermal and the buoyancy effect is not incorporated. Of course, for this case the Archimedes number is zero, and the thermal buoyancy is not a factor. The development of both numerical models, depends upon the assumption that the flows considered are inviscid. It is known that the viscous effects are inversely proportional to the Reynolds number. Since high Reynolds numbers are encountered in ventilation systems (in the range of 4,000 - 60,000 [4]) the inviscid approximation is justified. However, in boundary layers near walls, the viscous effects are significant and therefore the inviscid approximation breaks down leading to errors in the velocity predictions. Also, as a first approach to the ventilation problem, there was no account for viscous or turbulence effects. Recent investigations [5] suggest that no single turbulence model would guarantee a complete picture of the entire field. Therefore, in order to describe the airflow phenomenon in an air conditioned room, the air flow field should be divided into subfields, each having distinct physical characteristics (subfield modelling method, [6]), and the complexity of programming and operating the computer code would increase dramatically, beyond the scope of this thesis. Finally the 'primitive' set of equations (i.e. the equations for the u , v , P and not for the stream function and vorticity) is solved in

both codes, on a basis of the future development in 3-D, the immediate interest in the velocity variables, and the better physical understanding. Due to the simple geometry that is encountered in ventilation spaces, a Cartesian coordinate system was chosen, and a uniform grid with square mesh is used to simulate the physical domain, without the need of a more generalized coordinate system.

As it has been already mentioned, the two codes have some essential differences. The COMP code, which is presented in Chapter 2, is based on a finite difference formulation proposed by Rubin and Burstein [7]. It is an explicit, time-marching method that solves the hyperbolic type compressible fluid equations making use of the equation of state $\rho = f(P, T)$. The temporal derivative of density in the continuity equation enables the treatment of that equation as one in terms of a single dependant variable, i.e. density, from which the equation can be coupled to those of momentum. Of course, at low Mach numbers, the density and pressure become weakly related, and the variations of the latter become negligible. Despite this fact, examples can be found in the literature of applications of methods using the density as a dependant variable to practically incompressible situations [8]. Theoretically all flows are compressible and the pressure is always related to the density, no matter how weak their connection is.

When the second approach is used to formulate the INCOMP code, the air flow is considered incompressible and the density becomes completely decoupled from pressure. This fact presents some difficulties since neither an algebraic nor a differential equation is available for determination of pressure. But the continuity equation now assumes the role of a compatibility condition on the velocity field, leading to the determination of the pressure field, from an iterative solution sequence. Based on this concept, Patankar and Spalding [9] proposed a fully implicit upwind difference scheme, which is pursued in the formulation of the INCOMP code, and is described in detail in Chapter 3. A set of non-linear simultaneous equations is solved, but the implicit feature, which does not suffer from time-step restrictions, permits the direct calculation of the steady state solution.

Numerical results of the flow patterns in ventilated rooms with or without partitions, as obtained by the two codes are presented in Chapter 4. A discussion of

the results follows, and the numerical predictions are compared with experimental data, where possible. By doing so, the two codes and the validity of their assumptions can be tested. Finally, conclusions and recommendations for further work are made in Chapter 5.

1.2 Literature survey

1.2.1 Numerical methods

In this section a review is given of published work on numerical solutions, as applied to room ventilation. The study of air flows using numerical techniques has been done for more than twenty years, but only recently has a lot of activity been directed toward developing general fluid flow and heat transfer programs for solving the air flow in rooms.

In 1974, Launder and Spalding [10], proposed the k - ϵ turbulence model, which consists of a transport equation for the turbulent kinetic energy k , and an equation for the dissipation of turbulent kinetic energy ϵ . Turbulence is described by a 'turbulent viscosity', μ_t , and three equations with various constants describe the variables k , ϵ , and μ_t . This model formed the basis for most of the room flow programs currently in use. Nielsen [11], was the first who developed a calculation procedure for predicting two-dimensional, steady flow patterns in ventilated rooms. He adopted the k - ϵ model equations, and derived a numerical procedure based on the work of Gosman et al. [12] that solves for the vorticity, the stream function, the temperature and the two turbulent terms k and ϵ . The temperature difference between inlet and outlet is specified, and the predicted velocity and temperature distributions satisfactorily reproduce the experimental data. Since then, with the exception of Timmons [13], the stream function approach has been abandoned, in favor of the 'primitive variable' approach.

Timmons [13] developed an inviscid 2-D model, which solves for the vorticity and the stream function. Experimental findings by the same author [14], and the established jet theory, were the basis for determining functional relations for the

vorticity profile in a free jet, thus expressing the velocity equation as a Poisson equation. An iterative scheme is used to solve numerically for the vorticity, and short computational time is required for the convergence. For the cases considered, the numerical predictions produced reasonable correlations with experimental data. However, as Timmons noted, the code can not be modified to include obstructions in a room.

In 1977, Hjertager et al. [15], investigated the effect of the buoyancy forces in a numerical solution for 3-D room flows. The buoyancy term, in the form of Boussinesq approximation, appears in the momentum equation for the vertical velocity component, and the k and ϵ model equations are adopted. The numerical results were obtained by means of the SIMPLE algorithm [9, 49], and comparisons with experiments show that the agreement for isothermal flow is good. However, flow with buoyancy compares well with experiments in some regions and less well in others. Recent studies [16] show that the airflow in a room can be significantly affected by buoyancy for a corrected Archimedes number, Ar_c , greater than 75. Haghighat et al. [16], —apart from the v -momentum equation— incorporated two more terms in the k and ϵ equations, to account for the buoyancy effect. Very good agreement between the computed and the experimental Nusselt number was obtained. Buoyancy production terms in the k and ϵ equations were also studied by Chen et al. [17], for the flow simulation of natural convection in a cavity. The computations show that the influence caused by the buoyancy production terms (in the k and ϵ equations), is small with respect to the velocity and temperature profiles, but is significant in determining turbulence energy profiles. Similar numerical studies of buoyancy affected flows were also reported by Nielson et al. [18]. A 'primitive variable' approach was followed for a 2-D code, based on the Pope and Whitelaw two-equation turbulence model [19]. Initial wall jet development assumptions, based on experiments, were used for boundary conditions; and turbulent wall functions describe the near-wall regions close to all solid surfaces. The calculation procedure made use of the TEACH computer program devised by Gosman and Pun [20], and the necessity to include buoyancy terms in the k and ϵ equations for Archimedes numbers greater than 10^{-3} was demonstrated. Although

some discrepancies between numerical and experimental data occur, particularly in the area of reverse flow, the agreement is within 5% of the maximum velocity of the flow. The method was extended later to three dimensional flows [21]. Using the same numerical scheme as Nielsen, Reinhartz and Renz [22] investigated the flow in a rectangular room, ventilated by a diffuser for heating and cooling modes. The flow in a vertical plane of the room containing the diffuser, was well predicted by a 2-D solution.

Kato and Murakami [23], were the first to develop a 3-D code that allows the prediction of the velocity distribution and the spread of contaminants in downward flow clean rooms. The k and ϵ turbulence model [10] was used, and in addition to continuity, momentum and transport equations for k and ϵ , a contaminant transport equation was also solved. For the momentum equations, a centered difference scheme was adopted for both the convective and other terms, while for transport equations of scalar quantities (k , ϵ , and C) the QUICK scheme [24] was adopted. The general flow pattern and the contaminant concentration was satisfactorily predicted for six different air supply configurations. In further work, Murakami et al. [25] extended his code to account for the buoyancy effect, and the fluctuation of concentration, $\overline{c'^2}$. The equation which determined the fluctuation was not closed because a new variable, the dissipation rate of variance in gas concentration, appeared. The Zeman and Lumley model was used to close this equation. When the Reynolds number of the air flow at the inlet was large enough, the distributions of air velocity and mean concentration were well simulated by this code. This agreement did not arise when the Reynolds number was small. Recently [26] the code was modified to use generalized curvilinear coordinates instead of Cartesian.

Numerical investigations of velocity and temperature distributions in a room were also performed by Holmes [27], Markatos [28], Howarth [29], Jones and O'Sullivan [30], Whittle [31], and Awbi et al. [32, 33]. The common basis of all the above investigations was the PHOENICS computer code. PHOENICS is a general purpose, commercial computer code which was developed by Rosten and Spalding [34], for simulating fluid flow and heat transfer processes in engineering.

Recently, a cooling load program, the ACCURACY [35, 36], was developed in order to determine the boundary conditions for the PHOENICS code, such as wall surface temperatures, inlet air temperatures, etc. The ACCURACY code interacts with the PHOENICS code, since the outputs of the cooling load program can be used as inputs for the airflow program, and vice versa. Finally, this combination is used to study the influence of the indoor airflow and temperature distribution on room energy consumption, and evaluate ventilation efficiencies.

Unfortunately, the standard k and ϵ turbulence model [10], which is the cornerstone of the development of most of the room airflow programs to date, is suitable for high-Reynolds-number flows only. It cannot properly describe the airflow phenomenon in an airconditioned room, when the turbulent Reynolds number is low [37]. Since low Reynolds number turbulent flows, which include mixed convection, are reported in residential and office rooms [38], two alternative approaches are currently under development: The first is the adoption of a more complicated, nine-constant model, that allows consideration of laminar and low- turbulence flow [4]. The second is the division of the entire flow field into subfields, each having distinct physical characteristics [6]. Each subfield can be modeled individually, and the combination of all the subfield models provides a complete picture of the entire flow field.

1.2.2 Experimental investigations

The ability to predict the air movement in ventilated spaces does not rest merely on new airflow computer programs. There is also a need for high quality experimental data to assist physical understanding, and test the validity of the existing numerical codes. In this section, a brief review of experimental studies of air movement by forced or mixed convection is presented.

The first experimental investigations of the flow in air conditioned rooms (Millejaus [39], Urbach [40], Schwenke [41]), were mainly intended to provide support for simple design procedures, based on correlation equations. They made use of flow visualization techniques, were subject to unknown uncertainty in regions of

flow recirculation, and were mostly of a qualitative nature. Attempting to improve the accuracy of the measurements, Nielson et al. [3] made use of a laser - Doppler anemometry for his experimental investigations. Measurements obtained at Reynolds numbers between 5,000 to 10,000, showed that within experimental uncertainty, nondimensional velocity profiles were independent of Reynolds number for each geometry. For the same inlet geometry, longer rooms give rise to lower velocities, and for constant inlet velocity an increase of the area of the supply opening was accompanied by an increase of the maximum velocity in the reverse flow. The shape of the supply opening did not affect the nondimensional velocity profile. In further experimental work by Nielson et al. [18], the buoyancy effect was studied, and it was found that the maximum velocity in the reverse flow in a ventilated room, is determined by the heat load. Similar experiments by Awbi [42] showed that for isothermal flows the mean velocity is strongly influenced by the momentum of the supply jet, while as the cooling load increases, the influence of the jet momentum becomes less significant and the velocity is influenced by the convective currents created by the buoyancy forces in the room. Experiments on buoyant flows were also reported by Yamazaki et al. [43].

Pattie and Milne [2] investigated different types of air inlets in a scale model, by means of a chemical smoke. It was found that the airflow pattern is governed primarily by the configuration of the air inlet, while the Reynolds number had no significant effect on the flow pattern. Timmons [14] conducted experiments in small scale models and large prototype units, using small soap film bubbles and smoke. His measurements in the model and the prototype unit are in close agreement when geometric and dynamic similitude exists. For isothermal ventilated flows, a threshold Reynolds number was found (approximately 3,800) above which the dimensionless velocities and flow patterns are independent of changes in Re. More recently, Zhang et al. [5] conducted experiments in a model and a large scale room. The velocities were measured by a hot-wire anemometer, and smoke was used for flow visualization. Different types of subfields were observed in the airflow. It was discovered that under the presence of internal heat production, the air distribution was Reynolds number dependant. A similar relation was not observed

for isothermal and highly turbulent flow. The effect of the diffuser opening was also studied, and for the same ventilation rate the decrease of the diffuser opening resulted in higher velocities in the reverse flow region. Increasing the thermal buoyancy increased, linearly, the decay rate of the maximum velocity of the diffuser air jet.

Extensive experimental work on the air movement in connection with contaminant concentration distribution has been done for the last six years by Murakami et al. [23, 25, 26, 44]. A hot-wire anemometer, and a F.I.D. gas chromatograph were used for the measurement of the air velocity and the contaminant concentration respectively. One-sixth scale room models were used, and experiments conducted for thirteen different air supply outlets and exhaust inlet configurations. The influence of the arrangement of the supply inlet, and, to a smaller degree, of the exhaust outlets on the airflow distribution in a room, was confirmed. Moreover, it was found that the exhaust system was mainly responsible for the contaminant diffusion field. Similar experimental investigations and results on the contaminant concentration distribution in a ventilated room have been reported by Qingyan et al. [36].

Chapter 2

Compressible computer code

2.1 The numerical scheme

In the present analysis a two-step explicit and time-marching finite difference scheme is adopted to express the partial differential equations for the compressible flow. The finite difference formulations are given in Appendix A. However, some essential features of the numerical method are discussed here.

To analyze a two dimensional flow of an ideal gas, four dependant variables: two velocity components and any two other thermodynamic properties are required. For the compressible flow approach, the energy equation is coupled to the momentum and continuity equations, and there are four coupled differential equations to work with. When these differential equations are rearranged in a conservative form, they can be cast in a 'vector' form equation in the form:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0 \quad (2.1)$$

where the vectors $\mathbf{W}$, $\mathbf{F}$, and $\mathbf{G}$ are ordered sets of the variables ρ , ρu , ρv and ρe . Physically, $\mathbf{W}$ represents the quantity that may accumulate in the control volume, $\mathbf{F}$ the flux of $\mathbf{W}$ in the x direction, and $\mathbf{G}$ the flux of $\mathbf{W}$ in the y direction. For the inviscid case, neglecting the body forces, the Euler equations are obtained, and the matrices $\mathbf{W}$, $\mathbf{F}$ and $\mathbf{G}$ become:

$$\{W\} = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \end{Bmatrix} \quad \{F\} = \begin{Bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ (\rho e + P)u \end{Bmatrix} \quad \{G\} = \begin{Bmatrix} \rho v \\ \rho vu \\ \rho v^2 + P \\ (\rho e + P)v \end{Bmatrix}$$

For the solution of this matrix equation, Lax and Wendroff [45] proposed a forward time, centered space, finite difference formulation, which is second order accurate and diffusive. Based on this finite difference scheme, a considerable number of multi-step methods – which use the finite difference equations at split time levels – were developed, since it was noticed that they successfully simulate nonlinear hyperbolic equations. One of these schemes, the Rubin and Berstein scheme [7], was selected for the formulation of the compressible code. It is an explicit and time marching method, which is derived by applying a two step version of the Lax and Wendroff finite difference formulation, over half mesh increments $\frac{\Delta x}{2}, \frac{\Delta y}{2}, \frac{\Delta t}{2}$. This method uses forward time, centered space differences for the calculation of the first step, with the replacement of $W_{i,j}^n$ by its space average $\frac{1}{4}(W_{i-1,j}^n + W_{i+1,j}^n + W_{i,j-1}^n + W_{i,j+1}^n)$. The second step is a midpoint leapfrog calculation, which uses centered space and centered time differences. It is a predictor-corrector method, second order accurate both in time and space, that uses the temporary values of the dependant variables at the first time level $n + \frac{1}{2}$, for the computation of the final value at the second time level $n + 1$. The same finite difference equations of the Rubin and Berstein method can be derived by applying the conservation principles to each computational cell, which is treated as a finite control volume. The control volume approach, gives a better physical understanding of the finite difference expressions as well as the boundary conditions, and will be followed immediately.

The computational grid as shown in figure 2.1 is considered, with finite volume cells of dimensions Δx and Δy . Since the first step of the method is a half time, half space step, this implies that the values of the first step are centered on the boundaries between two cells, and are evaluated at half time of a step. Therefore, if a dependant variable is to be calculated at point (i, j) , then the same dependant

variable has to be calculated first at the points $(i + \frac{1}{2}, j + \frac{1}{2})$, $(i + \frac{1}{2}, j - \frac{1}{2})$, $(i - \frac{1}{2}, j + \frac{1}{2})$, $(i - \frac{1}{2}, j - \frac{1}{2})$, through the first step. Choosing the mass conservation equation as a model for all the conservation equations, its expression at the point $(i + \frac{1}{2}, j + \frac{1}{2})$ is:

$$\frac{\partial \rho}{\partial t} \Big|_{i+\frac{1}{2}, j+\frac{1}{2}} = - \frac{\partial(\rho u)}{\partial x} \Big|_{i+\frac{1}{2}, j+\frac{1}{2}} - \frac{\partial(\rho v)}{\partial y} \Big|_{i+\frac{1}{2}, j+\frac{1}{2}} \quad (2.2)$$

The advective flux of mass into the control volume of figure 2.2 has four components: two in the x direction (through the points (i, j) and $(i + 1, j)$), and two in the y direction (through the points (i, j) and $(i, j + 1)$). Similarly there are four advective fluxes of mass out of the control volume, through the points $(i, j + 1)$ and $(i + 1, j + 1)$ for the x direction, and $(i + 1, j)$, $(i + 1, j + 1)$ for the y direction. Summing all the fluxes properly multiplied by the corresponding area and the time interval, will account for the total increase of the mass in the control volume during the time interval $\frac{\Delta t}{2}$, i.e. the expression of the first term in equation (2.2). Then the equation (2.2) becomes:

$$\begin{aligned} \{ \rho \Big|_{i+\frac{1}{2}, j+\frac{1}{2}}^{n+\frac{1}{2}} (\Delta x \Delta y) - \rho \Big|_{i+\frac{1}{2}, j+\frac{1}{2}}^n (\Delta x \Delta y) \} &= \frac{\Delta t}{2} \{ (\rho u)_{i,j}^n \frac{\Delta y}{2} \\ &+ (\rho u)_{i+1,j}^n \frac{\Delta y}{2} + (\rho v)_{i,j}^n \frac{\Delta x}{2} + (\rho v)_{i,j+1}^n \frac{\Delta x}{2} - (\rho u)_{i+1,j+1}^n \frac{\Delta y}{2} \\ &- (\rho u)_{i,j+1}^n \frac{\Delta y}{2} - (\rho v)_{i+1,j}^n \frac{\Delta x}{2} - (\rho v)_{i+1,j+1}^n \frac{\Delta x}{2} \} \end{aligned} \quad (2.3)$$

Dividing both sides by the finite area $\Delta x \Delta y$, and replacing the value of the dependant variable at point $(i + \frac{1}{2}, j + \frac{1}{2})$ and at time n , by its space average $\frac{1}{4}(\rho_{i,j}^n + \rho_{i,j+1}^n + \rho_{i+1,j}^n + \rho_{i+1,j+1}^n)$, equation (2.3) is written as:

$$\begin{aligned} \rho_{i+\frac{1}{2}, j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}(\rho_{i,j}^n + \rho_{i,j+1}^n + \rho_{i+1,j}^n + \rho_{i+1,j+1}^n) + \frac{\Delta t}{\Delta x} \frac{1}{4} [(\rho u)_{i,j}^n + (\rho u)_{i+1,j}^n - (\rho u)_{i,j+1}^n \\ &- (\rho u)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4} [(\rho v)_{i,j}^n + (\rho v)_{i,j+1}^n - (\rho v)_{i+1,j}^n - (\rho v)_{i+1,j+1}^n] \end{aligned} \quad (2.4)$$

Similarly expressions for the other three half space points adjacent to (i, j) can be derived.

Using the density at the surrounding four half space nodes, computed at time $n + \frac{1}{2}$, along with the density at the grid point (i, j) obtained from the previous

time step, the computation of the density for the full time step Δt follows:

$$\begin{aligned} \rho_{i,j}^{n+1} = & \rho_{i,j}^n + \frac{\Delta t}{\Delta x} \frac{1}{2} [(\rho u)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho u)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho u)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] \\ & + \frac{\Delta t}{\Delta y} \frac{1}{2} [(\rho v)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho v)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] \end{aligned} \quad (2.5)$$

For stability reasons, an effective mass diffusion type damping term was implemented in the full time step in the same form as it was proposed by Yoshihara [46]. For any property that is computed at the node (i,j) at time $(n+1)$, the value at time n is replaced by a combination of this value at time n , and the values in the four neighboring nodes of this node. Then, in equation (2.5) the term $\rho_{i,j}^n$ is substituted by the expression: $(1-F_x-F_y)\rho_{i,j}^n + 0.5F_x(\rho_{i,j+1}^n + \rho_{i,j-1}^n) + 0.5F_y(\rho_{i+1,j}^n + \rho_{i-1,j}^n)$. The constant multipliers F_x and F_y that correspond to the x and y directions, can be adjusted to result in the proper amount of diffusive damping needed.

The CFL stability criterion established by Courant, Friedrichs and Levy, was adopted to determine the allowed time step during the computations. According to Roache [47], for a 2-D solution, the CFL criterion, which requires that the continuum information speed is less than or equal to the computational information speed, is given by:

$$\Delta t \leq \frac{1}{\sqrt{2}} \frac{\Delta x}{(|u| + c)}, \frac{1}{\sqrt{2}} \frac{\Delta y}{(|v| + c)}$$

where c is the local sound speed.

2.2 Boundary conditions

For a first order hyperbolic equation, one initial condition needs to be specified. Therefore an initial distribution of the dependant variables ρ , ρu , ρv and ρe in the computational domain is required. Moreover, boundary conditions at the inflow, outflow and solid walls have to be prescribed [48]. Since a rectangular type computational domain simulates the physical domain, the grid points may be specified as coincident with the boundaries of the physical domain, thus making specification of boundary conditions less complex. The grid points on the boundaries of the

solid walls can be either half step or full step points, since, regardless of which of these chosen, no difference in the numerical results was noticed. Contrarily, only the selection of the full step points placed as grid points on the inflow and outflow boundaries, ensures stability and convergence.

There are two different approaches for the derivation of the solid wall slip boundaries: The first is the 'reflection' method, where an extra line of fictitious points inside the wall is defined, as in figure 2.3. Then fictitious values are defined at the points $(i - \frac{1}{2}, j - \frac{1}{2})$, $(i - \frac{1}{2}, j + \frac{1}{2})$, by antisymmetric reflection of the normal velocity component at the wall and symmetric reflection of the other variables:

$$v_{i-\frac{1}{2},j} = -v_{i+\frac{1}{2},j}, \rho_{i-\frac{1}{2},j} = \rho_{i+\frac{1}{2},j}, u_{i-\frac{1}{2},j} = u_{i+\frac{1}{2},j}, e_{i-\frac{1}{2},j} = e_{i+\frac{1}{2},j}$$

The flow parallel to the wall at the point (i, j) is satisfied, and regular interior point differencing can be used. The other approach is the finite volume approach, where the only condition to be satisfied is the flux of all transported properties across the wall to be zero. With reference to figure 2.3 and considering the fact that the control volume of the grid point (i, j) has half the size of a regular one, the full time step equation of conservation of mass yields:

$$\begin{aligned} \rho_{i,j}^{n+1} = \rho_{i,j}^n &+ \frac{\Delta t}{\Delta x} [(\rho u)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] \\ &+ \frac{\Delta t}{\Delta y} [-(\rho v)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] \end{aligned} \quad (2.6)$$

The same formula applies for the u velocity component, and the energy at the point (i, j) , while the v velocity component is assigned a zero value. Similarly for the case of a grid point located at the corner, as in figure 2.4, the control volume is one fourth of the size of a regular one. Both u and v velocity components are zero, and only the equations of mass and energy conservation are solved. Hence, the density at (i, j) becomes:

$$\rho_{i,j}^{n+1} = \rho_{i,j}^n + 2 \frac{\Delta t}{\Delta x} [(\rho u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] + 2 \frac{\Delta t}{\Delta y} [-(\rho v)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] \quad (2.7)$$

For the inflow boundary, the values of the dependant variables are prescribed, and the air velocity is considered to be uniformly distributed over the entire area of the supply opening.

Different linear extrapolations of the flow property variation within the computation field to the cell located just outside the region of computation, were applied to the outflow boundary. The quadratic and cubic extrapolations of the forms $f_{i,j} = 3f_{i,j-1} - 3f_{i,j-2} + f_{i,j-3}$, $f_{i,j} = 4f_{i,j-1} - 6f_{i,j-2} + 4f_{i,j-3} - f_{i,j-4}$ as well as the form $f_{i,j} = 2f_{i,j-1} - f_{i,j-2}$, where $f = \rho, u, v, T$ were tested for a simple pipe case. It was found that they would not provide convergence except for a few special conditions (certain inlet velocity, length of the pipe). Instead, another approach was used: Consider the schematic representation of the first and second step for a 1-D case as can be seen in figure 2.5.a. If the advection terms of the grid points located at the outflow boundary, are evaluated by upwind differencing, then the schematic representation of figure 2.5.b results, and the equation of the full time step for the density at an outflow grid takes the form:

$$\rho_i^{n+1} = \rho_i^n + 2 \frac{\Delta t}{\Delta x} [(\rho u)_i^n - (\rho u)_{i-\frac{1}{2}}^{n+\frac{1}{2}}] \quad (2.8)$$

By this approach, convergence is achieved for a simple pipe case, regardless of the inlet velocity or the length of the pipe. However, for some 2-D geometries, computational stability has to be imposed by defining the outlet pressure. This is permitted, since the outflow is subsonic [48]. Well defined outflow boundary conditions are always the case in numerical simulations of ventilation systems, and some researchers suggest that it is a necessary condition for a reliable solution to be achieved [32, 33]. The specification of the outflow boundary was found desirable, in order to reduce the excessive computational time needed for achieving the asymptotic steady state flow field, due to the small allowable time step.

Lastly, the sharp convex corner type of boundary required special treatment. Initially, the control volume approach was applied to the sharp corner of figure 2.6, where a grid point is located exactly at the edge of the corner. Then the size of the control volume for the point (i,j) is three-quarters of the size for a regular one, and a new set of finite difference equations is derived. But even for small mesh size and large diffusive damping coefficients, this approach leads to computational instabilities. Next, the method of double-valued treatment of a fictitious inner value at $(i + \frac{1}{2}, j + \frac{1}{2})$ was pursued, without achieving stability.

Instabilities were also encountered using the method of discontinuous values at the point (i,j) . Finally, it was decided to avoid assigning a node point at the sharp corner, but rather to place node points only in the vicinity of it. Additionally, the mesh size was decreased, making convergence and stability feasible even for very low diffusive damping coefficients.

2.3 Main features of the COMP code

Based on the finite difference equations of appendix A, and the treatment of boundary and initial conditions as it is discussed in the previous section, the computer program COMP was developed in FORTRAN-77 programming language. The structure of COMP is represented by the flow chart given in figure 2.7.

The main program consists of three parts: the initial conditions, the geometric data and the fluid properties data. For the prescription of the initial boundary conditions, values of the density, the two velocity components and the temperature are defined for the whole computational domain. These are the conditions at time zero, through which the internal energy per unit mass, and eventually the total energy per unit volume can be obtained. The geometric data define the mesh sizes Δx and Δy , the dimensions of the space to be ventilated, of the inlet and outlet, and of any partitions if they exist. Calculation of the grid structure follows the input of these data. The fluid properties data (the fluid medium is air) provide information for the gas constant and the two specific heat coefficients which are considered constant. Making use of these data, the initial maximum allowable time step can be calculated. Finally, values for the diffusive damping coefficients are assigned, and a flag for convergence inspection is created, along with an output file that permits vectors of the resulting velocities to be plotted. In the main program, three subroutines are called: STEP1, STEP2, and UPDATE.

In STEP1, the half time, half space flow values are calculated, by calling a series of subroutines that solve the equations for regular and boundary cells. The solution sequence in each of these sub-subroutines, involves first computing the density, followed by the two momentum equations, from which the velocity components

are deduced when divided by the density. Next, the total energy is derived from the energy conservation equation, and through it, the pressure is computed in order to be used in the next cycle. The expression for the pressure can be found using the state equation $\rho = \frac{P}{RT}$, the total energy equation $e = c_v T + \frac{1}{2}(u^2 + v^2)$ and the two relations that connect the ratio of the specific heats with the gas constant; $\gamma = \frac{c_p}{c_v}$, $c_v = c_p - R$. Combining the above equations, the pressure is given by

$$P = [e - \frac{1}{2}(u^2 + v^2)](\gamma - 1)\rho \quad (2.9)$$

In STEP2, using the values obtained in STEP1, the flow values at the full time step nodes are calculated. A separate subroutine is used for each cell type, and the full time equations as given in Appendix A are solved. The solution sequence is the same as was followed in STEP1.

Finally, in UPDATE, the new full time values that were calculated in STEP2, replace the old full step values and become the new initial condition for the next cycle, thus terminating one cycle. Consequently, the use of a two step method allows for only two levels of values to be stored at any time: the half time and full time flow property values. Since the old value for both steps is no longer needed when the new value has been computed, the new value is written over the old one to conserve in storage space. Moreover, in UPDATE, the new calculated values are checked for any unrealistic results (e.g. negative density) and if so, a message is printed and the program terminates. The highest value of the two velocity components is also found, and is used for the calculation of the allowable time step for the next cycle. By this way, a time marching procedure is obtained, allowing the prediction of the steady state flow field.

2.3.1 Simple test cases

The computer code COMP, was first tested for two simple geometries, a simple pipe and a corner pipe. Useful information was obtained from these simple cases. First, parametric numerical investigations were made for a simple pipe case. It was found that if half time node points are assigned at the outflow boundary, growing

oscillations appear, and the numerical scheme is unstable. This behavior changes when full time steps are located at the outflow boundary, but the numerical scheme becomes subject to instabilities for a range of time steps and diffusive damping coefficients, when no outflow boundary condition is prescribed. If Δt is the maximum allowable time step because of the CFL criterion, then independently of the inlet velocity, the numerical scheme provides convergence for an optimum range of time steps, which are confined between $0.3\Delta t$ and $0.6\Delta t$. If the time step for every cycle is less than $0.3\Delta t$, the solution diverges. If it is more than $0.6\Delta t$, the solution converges at a very slow rate. The above remarks, are valid for zero diffusive damping. If diffusive damping is applied, it damps out the oscillations obtained with small time steps, and provides stability. Figures 2.8.a, 2.8.b, 2.8.c and 2.8.d show the behaviour of the numerical scheme for two different inlet velocities, using different time steps, and varying the diffusive damping coefficient denoted as F_z , from zero to 0.05.

For the corner pipe case, similar sensitivity of the numerical scheme with the time step and the diffusive damping coefficients made it necessary to prescribe the outflow pressure. Figure 2.9 shows the velocity field that was obtained by specifying the outflow pressure. The optimum time step, the mesh size and the diffusive damping coefficients are again interrelated. A small mesh size is required in order for the diffusive damping coefficients to be minimized and not cause the smearing of the real flow. As a result of this, the corresponding allowable time step decreases, and the total computational time increases. For the velocity field of figure 2.9, the mesh size for both dimensions was 0.1m, while the diffusive damping coefficients were both equal to 0.01, which is a very satisfactory value.

Chapter 3

Incompressible computer code

3.1 The numerical scheme

In this section, the main features of the numerical method that forms the basis for the development of the INCOMP code are presented. The fundamental equations which govern the flow characteristics of a general 2-D, isothermal, inviscid, incompressible fluid flow for a steady state, are the following conservation equations of mass and momentum:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0 \quad (3.1)$$

$$\frac{\partial(\rho u u)}{\partial x} + \frac{\partial(\rho v u)}{\partial y} = -\frac{\partial P}{\partial x} \quad (3.2)$$

$$\frac{\partial(\rho u v)}{\partial x} + \frac{\partial(\rho v v)}{\partial y} = -\frac{\partial P}{\partial y} \quad (3.3)$$

The equations (3.1) to (3.3) contain three unknowns: Two velocity components and the pressure. A procedure for solving the differential equations (3.1) to (3.3) is to integrate them over finite control volumes which constitute the calculation domain. Then, the equations are represented in discretized form, and the velocity components and fluid properties are computed at specific locations on a mesh of

grid nodes within the flow domain. At this point, a staggered grid arrangement as shown in figure 3.1 is introduced. The reasons for adopting the staggered grid are for simplicity in applying the pressure gradient terms in the momentum equations and in specifying the special form of the mass conservation equation. The pressure and density control volumes are the ones centered on grid nodes such as P in figure 3.1. The velocity components u and v which lie between the pressures driving them, are displaced in the x and y directions respectively, to the midpoint of the boundaries of the control volumes surrounding the scalar quantities pressure and density. Each variable then is assumed to have its own grid and finite volume, that is, the grid points for the velocity components u and v are located at the centers of the volume for which the pressures are obtained at the boundary surface. The momentum control volumes are defined around the velocity location.

Consider the u -momentum control volume which is split between two half-pressure volumes, as it is shown in figure 3.2. The u_P location is defined exactly midway between the grid points w and e for pressure. By integrating the equation (3.2) over the control volume, and using central differences, it follows:

$$\Delta y\{(\rho u)_e u_e - (\rho u)_w u_w\} + \Delta x\{(\rho v)_n u_n - (\rho v)_s u_s\} = \Delta y(P_w - P_e) \quad (3.4)$$

Since no diffusion terms exist, an upwind scheme is adopted. Then, the value of the u component at an interface is equal to the value of the u component at the grid point on the upwind side of the face. The equation (3.4) is transformed into:

$$\begin{aligned} & (\Delta y\{[-(\rho u)_e, 0] + [(\rho u)_w, 0]\} + \Delta x\{[-(\rho v)_n, 0] + [(\rho v)_s, 0]\})u_P = \\ & = \Delta y\{u_E[-(\rho u)_e, 0] + u_W[(\rho u)_w, 0]\} + \Delta x\{u_N[-(\rho v)_n, 0] + u_S[(\rho v)_s, 0]\} \\ & + \Delta y(P_w - P_e) \end{aligned} \quad (3.5)$$

where the symbol $[]$ stands for the largest of the quantities contained within it. The discretization equation (3.5) can be written in a compact form as:

$$a_P u_P = a_E u_E + a_W u_W + a_N u_N + a_S u_S + (P_w - P_e)A_P \quad (3.6)$$

where a_i are the neighbor coefficients representing the convection flux at the cell boundary surfaces, and A_e is the area over which the pressure difference acts. The

subscripts E, W, N, S represent the neighbor grids of grid P, as shown in figure 3.2. The mass flow rates at the boundaries of the control volume, are evaluated by averaging the neighboring nodal values, e.g. the mass flow rate $(\rho u)_e$ is taken to be $\frac{1}{2}((\rho u)_P + (\rho u)_E)$. The finite volume equations for the other velocity component v , can be solved in a discretized form following a similar procedure. Then, for the finite control volume of figure 3.3, the v_1 component of velocity is given by:

$$\begin{aligned}
 & (\Delta x \{ [-\frac{1}{2}((\rho v)_1 + (\rho v)_3), 0] + [\frac{1}{2}((\rho v)_1 + (\rho v)_3), 0] \} \\
 & + \Delta y \{ [-\frac{1}{2}((\rho u)_9 + (\rho u)_8), 0] + [\frac{1}{2}((\rho u)_7 + (\rho u)_6), 0] \}) v_1 = \\
 & = \Delta x \{ v_3 [-\frac{1}{2}((\rho v)_1 + (\rho v)_3), 0] + v_2 [\frac{1}{2}((\rho v)_1 + (\rho v)_3), 0] + (P_{10} - P_{11}) \} \\
 & + \Delta y \{ v_5 [-\frac{1}{2}((\rho u)_9 + (\rho u)_8), 0] + v_4 [\frac{1}{2}((\rho u)_7 + (\rho u)_6), 0] \} \quad (3.7)
 \end{aligned}$$

By this procedure, discretization equations of finite difference form are obtained for all the nodal points for the two velocity components, on a computational grid superimposed over the physical domain. Since the resulting momentum equations for all the grid points are nonlinear and interlinked, we cast them into nominally linear form by calculating tentative values of the coefficients for an initial guessed velocity field. Then, the discretized equations are solved repeatedly with updated coefficients. Since a repetitive solution of the algebraic equations is needed in order to handle the nonlinearity, iterative rather than direct methods are adopted. The main disadvantage of the direct methods is that they are much more complicated and require rather large amounts of computer storage and time. From the iterative methods, the Gauss-Seidel point-by-point and line-by-line methods were used. In the former, the values of the velocity variable are calculated by visiting each grid point in a certain order. The temporarily known values are taken from the most recently calculated values, and when all grid points have been visited, one iteration is complete. In the latter method, the same 'visiting' principle applies, but a line rather than a point is visited at a time. By assuming that the velocity values on the neighbouring lines are known from the most recently calculated values, a tri-diagonal matrix is formed, and is solved by applying the Thomas algorithm. Adjacent lines are treated in a similar fashion, and the whole flow domain is swept

in this manner. To ensure stability and convergence, under-relaxation is employed for both methods. The calculated velocity components satisfy the momentum equations for a guessed pressure field, but do not in general satisfy the local mass balance. To overcome this difficulty, the SIMPLE algorithm which was described by Patankar [49] is followed, and its main features are given below.

Since the pressure field is not known, it must be computed by an iterative 'guess and correct' procedure. Denoting by u^* , v^* the resulting velocity field based on a guessed pressure field P^* , simultaneous corrections should be made to both fields to cancel the mass imbalance. For this, the local pressure correction P' is

$$P = P^* + P' \quad (3.8)$$

Then, the velocity corrections are assumed to depend upon pressure corrections changes, and are given for example by

$$u_P = u_P^* + u_P', \quad u_P' = \frac{A_P}{a_P} (P'_w - P'_e) \quad (3.9)$$

with reference to equation (3.6). If the mass conservation equation (3.1) is integrated over the finite control volume of figure 3.4, it yields:

$$\rho \{ (u_P - u_w) \Delta y + (v_N - v_s) \Delta x \} = 0 \quad (3.10)$$

Substituting the velocity expressions as in equation (3.9) to (3.10) it follows:

$$\begin{aligned} & P'_1 \rho \left\{ \frac{A_P}{u_P} \Delta y + \frac{A_w}{u_w} \Delta y + \frac{A_N}{u_N} \Delta x + \frac{A_s}{u_s} \Delta x \right\} = \\ & = \rho \left\{ P'_2 \frac{A_P}{u_P} \Delta y + P'_3 \frac{A_w}{u_w} \Delta y + P'_5 \frac{A_N}{u_N} \Delta x + P'_4 \frac{A_s}{u_s} \Delta x \right. \\ & \left. + (u_w^* - u_P^*) \Delta y + (v_s^* - v_N^*) \Delta x \right\} \end{aligned} \quad (3.11)$$

The equation (3.11) is solved for P' at each grid node for pressure, using the Gauss-Seidel line-by-line method. Then, the pressure field and the velocity components are updated, by the equations (3.8) and (3.9), and the corrected pressure field is used as a new guessed pressure field to solve the set of the momentum equations. This iterative procedure is repeated until the continuity of flow for

every control volume has been achieved to a specified tolerance. Synoptically, the steps of the SIMPLE algorithm are as follows:

1. Guess the pressure field P^* .
2. Solve the momentum equations, such as equations (3.5) - (3.7) to obtain u^* and v^* .
3. Solve the P' equation (3.11).
4. Calculate P from equation (3.8)
5. Calculate u and v from their starred values using the velocity-correction equations (3.9)
6. Treat the corrected pressure P as a new guessed pressure P^* , return to step 2, and repeat the whole procedure until a converged solution is obtained.

Finally, it should be emphasized that for complex flows, a situation may arise where all the mass flows exit from a control volume. In this case, the finite volume equation of the momentum for inviscid steady state flows becomes singular. To remedy this problem, either the values of the under-relaxation factors should change during the iterative procedure, or a 'false' source term S_f should be added to equation (3.6) [50]. The source term is defined as $S_f = C_P(u_P^{i-1} - u_P^i)$, where

$$C_P = | \dot{m}_n - \dot{m}_s + \dot{m}_e - \dot{m}_w | \quad (3.12)$$

The superscript i denotes the i 'th iteration in the solution of the momentum equation. The form of the final finite volume equation for momentum then becomes:

$$(a_P + C_P)u_P^i = a_E u_E + a_W u_W + a_N u_N + a_S u_S + (P_w - P_e)A_P + C_P u_P^{i-1} \quad (3.13)$$

While the addition of the false source term stabilizes the solution procedure, it has no effect on the final solution.

3.2 Boundary conditions

The numerical scheme that was described in the previous section, requires the prescription of the inlet, outlet and wall boundary conditions. The computational grid is arranged so that the boundary finite volumes for pressure and the physical domain boundaries coincide, and thus the boundary grid points of the velocity are placed on the outer surfaces of the boundary finite volumes as in figure 3.5. With this arrangement, conservation is ensured over the entire domain, and the boundary conditions enter naturally.

At the inlet, the velocity is specified, and uniform distribution is assumed over the whole inlet boundary.

At the exit, either the pressure or the outlet velocity should be prescribed. When the outlet velocity is prescribed, it can be derived from the continuity equation, and uniform distribution is assumed across the exit area. When the exit pressure is prescribed, for the inviscid case, it can be assigned the zero value. Regarding the pressure field, it is only the relative pressure within the flow domain which is important. It is therefore permitted to fix a reference pressure (in this case the exit pressure) and compute pressures elsewhere based on the pressure gradients. Since the density is assumed unaffected by pressure, pressure is then a relative variable and not an absolute one. The need for boundary values of the velocity downstream of the calculation domain is also eliminated, due to the upwind differencing. Since the region near the outflow boundary exhibits for large Peclet numbers, local one-way behaviour, for all the grid points next to the outflow boundary the coefficients a_E will be zero. The only restriction for the above reasoning is that the outflow boundary is placed at a proper location, where no 'inflow' is expected. Moreover, when the exit pressure is given, the value of the pressure correction P' at the exit is zero, and the pressure correction equation should not be solved for the outflow grid point.

For the wall boundary, the only requirement is to ensure that the normal velocity across the wall is zero. Using the computational grid of figure 3.5, this can be done by setting the relevant coefficients to zero, while solving the momentum

equations (e.g. $\alpha_N = 0$ for cell adjacent to a 'north' boundary, $\alpha_E = 0$ for cells next to an 'east' boundary and so on). The specification of the velocity at the wall boundary affects also the pressure correction equation. With reference to figure 3.6, the flow rate across the east boundary face is not expressed in terms of u_e^* and a corresponding correction, but in terms of u_e itself. Then no information about P'_E is needed, and P'_E does not appear in the pressure correction set of equations.

3.3 Main features of the INCOMP code

The purpose of this section is to describe the principles of organization and structure of the INCOMP code for isothermal and incompressible flows. Also included is a description of the functions of the individual subroutines. Based on the numerical scheme of the previous section, the INCOMP code was developed in FORTRAN-77 programming language. The program was written in a relatively straightforward form, which is readily amenable to modifications. Figure 3.7 shows the structure of the INCOMP code in flow chart form.

The program starts by specifying geometric data. The mesh sizes Δx , Δy , and the dimensions of the room, its inlet and outlet, are defined. The computational grid is then derived, using the above data.

Next, the boundary conditions are given. Either the outlet velocity or the exit pressure, together with the inlet velocity and the location of the walls and any obstacles are determined. The air density is also given, since it is the only necessary fluid property to be defined.

The third part of the input data, provides the under-relaxation factors for the momentum and pressure correction equations, and the convergence criteria upon which the convergence of the iterative Gauss-Seidel procedure is judged. Because only tentative coefficients are used, special attention should be given to the choice of the convergence criteria. The iterative solution of the algebraic equations need not be taken to complete convergence, and a maximum number of iterations is prescribed. If the iterative procedure requires more iterations than the prescribed maximum value in order to satisfy the convergence criteria, the program stops

and a message to change these criteria is printed. Finally, a flag for convergence inspection of the overall algorithm is created. The solution is assumed to have converged when the sum of the absolute mass residuals of all the finite volumes, has fallen below a specified level ϵ . Optional flags are also available, to enable the user to obtain the values of the dependant variables at each of the nodal points of the computational grid, at any desired iteration level. These values can be printed on an output file, together with the final converged velocity values.

The calculating procedure starts by initializing the fields of the two velocity and pressure variables. Then, the discretized coefficients of the momentum equations are assembled, and they are transferred to the VELOCITY subroutine, which is then called. The VELOCITY subroutine, uses the calculated coefficients to solve the linearized equations for the velocity components, through the point or line-by-line Gauss-Seidel method. When the convergence criterion for the iterative solution is satisfied, new velocity coefficients, based on the last calculated values of velocity are computed. The updated coefficients are transferred back to the main program and they are compared with the old ones. If the absolute value of the difference between them, is larger than a specified level, then a loop is entered between the main program and the VELOCITY subroutine, until the specified difference level is satisfied.

Next, the coefficients for the pressure correction equations are calculated and they are transferred to the PRESSURE subroutine, which is called. In the PRESSURE subroutine, the line-by-line Gauss-Seidel method is incorporated to solve the linear set of the pressure correction equations. Once convergence has been satisfied in the iterative method, the calculated values of pressure correction are transferred back to the main program. Using the correction equations, appropriate corrections to pressure and velocity components are made. The old pressure and velocity values are over-written by the present ones, which are used to reinitialize the velocity and pressure fields.

At this stage of the program, the mass residual for each finite volume is computed, and the sum of their absolute values is checked against the convergence criterion ϵ . If convergence is satisfied, the program terminates by writing all the

information sought for, in the output file. Otherwise a new iteration loop of the calculating procedure begins, by calculating new velocity coefficients and so on. The loop is repeated, until it is exited when the procedure converges.

3.3.1 Simple test cases

Similarly to the COMP code case, the INCOMP code was first tested for two simple geometries: a simple pipe and a corner pipe. The conclusions derived from the two tests will be briefly discussed below.

For both tests, the solution was assumed to be converged when the sum of the absolute mass residuals of each control volume, was less than 0.1% of the total inlet mass flow applied at the boundary of the domain of calculation. For the 1-D, simple pipe case, the line-by-line Gauss-Seidel method, degenerates to the TDMA (Tridiagonal-Matrix-Algorithm). Therefore, the TDMA method was used for solving the pressure correction set of equations, while for the momentum equations, the TDMA and the point Gauss-Seidel methods were used alternatively. No significant difference in the computing time was noticed between the two methods.

Parametric investigation was conducted for the convergence criteria of the iterative methods, the under-relaxation factors, and the initial guess of the velocity fields. Though the computing time was not large enough for quantitative observations, the following qualitative observations were made: The closer the initial guesses of the distributions of the variables are to the final solutions, the fewer will be the iterations required to reach the solutions. Lower values for the under-relaxation factors result to more iterations for the final solution, and consequently more computing time. Lower values for the convergence criteria of the iterative methods result in fewer iterations, but will increase the computing time per iteration, so an optimum exists.

It was also noticed that instability may arise from bad specification of the initial field of pressure or velocity, from inappropriate choice of under-relaxation factors, and from bad selection of convergence criteria. The above three factors for instability are also closely related to the minimization of the computing time.

The need for lower under-relaxation factors and convergence criteria to reassure convergence, contradicts the necessity for high as possible values to minimize the computing time, especially in complex 2-D flows. Since there are no general rules for choosing the best factors, 'trial and error' procedure and exploratory computations are necessary for finding the optimal values.

For the 2-D, corner pipe test, the above speculations were verified, and the influence of the under-relaxation factors, the convergence criteria, and the initial field guess on the computing time, became more intense. Moreover, the influence of the mesh size was studied. Figures 3.8.a and 3.8.b, show the resulting velocity field for mesh sizes $\Delta x = \Delta y = 0.4\text{m}$ and $\Delta x = \Delta y = 0.2\text{m}$ respectively. No significant changes are observed, but the computing time in the second case is much larger. Therefore, a compromise between the fineness of the computational grid and the required computing time is desirable.

Two exit boundary conditions were tested. In figure 3.8.c the exit pressure was prescribed, while in figures 3.8.a and 3.8.b the exit velocity was prescribed, and the outflow boundary was moved further downwards in order to make the assumption of the uniformness of the outlet velocity safe. No changes in the resulting velocity fields occurred. Finally, the influence of the inlet velocity was examined, and it was calculated that the overall computing time is not affected by it, when the rest of the parameters are kept constant.

Chapter 4

Results and discussion

A major part of this study has been the development of the two computer codes which were discussed so far. Once the codes were developed, different cases of ventilated rooms were studied, by varying the length L and height H of the room, the configuration of the exhaust and supply system, and the Reynolds number¹. Also, cases with two and three workstations, separated by one and two partitions respectively were investigated, first with partitions set on the floor and then by raising the partitions, or removing a part of them from the bottom. In all cases, the convergence criterion for the INCOMP code was satisfied when the sum of the absolute mass residuals of each control volume was less than 1% of the total inlet mass flow. For the COMP code, convergence was achieved when the sum of the absolute differences of the old and new time step velocities, was less than 0.01. The mesh sizes used in the majority of the numerical studies, were either 0.2 or 0.1m for both codes. The required computing time for convergence, was mainly a function of the geometric characteristics, apart from any particular features that the code exhibits as they were discussed in sections 2.3.1 and 3.3.1. In general, when the same mesh size was used, the computing time required by the INCOMP code, was approximately one order of magnitude less than that required by the COMP code.

¹Reynolds numbers are based on the inlet velocity and the slot width.

To check the validity of the numerical predictions, it was essential to test them against some flow patterns in ventilated rooms for which experimental results are available. Unfortunately, such results are limited, since a significant part of the experimental data for ventilated rooms has been derived from natural convection driven flows, or flows where large temperature gradients are present; consequently they are not suitable for comparison with the cases that can be computed. Similarly, data based on airflows with three-dimensional effects, are not suitable for comparison with the current 2-D code predictions; a 3-D model would be required to produce comparable results.

In the following sections of this chapter, the numerical results are discussed, with the necessary geometric, flow, and computational characteristics of the cases presented in sections 4.1, 4.2.2 and 4.2.3, given in tables 1, 2, and 3 respectively. Moreover, velocity vector plots were used for illustration of the predicted flow patterns. The magnitude of each vector corresponds to a nondimensionalized velocity, obtained with respect to the maximum velocity appearing in the flow field. In all the plots, the minimum relative velocity value plotted, was 0.1–0.01.

4.1 Partitionless ventilated rooms

This section presents the numerical predictions and the experimental data for ventilated rooms with no solid obstacles. The first case that was studied simulated the flow field observed in Timmons' experiment [14]. In his full scale model experiment, Timmons enforced a two dimensional behaviour at the midplane where velocity data were collected, using an inlet aspect ratio² greater than 20. The air-flow is discharged from the left side wall, and is drawn into an inlet placed on the opposite wall. The measurements were obtained for Reynolds number 1.8×10^4 , and the geometric and dynamic features of the experiment were reproduced in the simulations. Figures 4.1.a and 4.1.b, show the simulated flow patterns derived from the INCOMP and COMP code respectively. Figures 4.2.a, 4.2.b and 4.2.c

²Aspect ratio is the ratio of slot length to slot width.

show the comparison between the experimentally obtained dimensionless velocity profiles, and the numerically predicted ones.

The next case that was examined, was based on the experimental studies by Nielsen et al. [3, 11]. Nielsen conducted his experiments in a small scale model, and verified his results in a full scale test room. In the experimental set up, the air is supplied by a slot diffuser along the ceiling, from one end of the room, while the outlet slot is located at the bottom of the opposite end of the room. The width of the inlet and outlet slot is equal to the width of the room, thus limiting any three-dimensional effects. For the numerical investigations, the inlet and outlet configuration was reproduced, together with the Reynolds number that was fixed at 9.5×10^3 . Also, all the non-dimensional geometric quantities were maintained in order to satisfy geometric similitude. The experimentally derived normalized velocity profile in the centerline of the model, measured at a distance of $\frac{1}{3}L$ from the inlet slot, is compared with the numerical predictions in figure 4.3. Figures 4.4.a and 4.4.b show the airflow field as predicted by the INCOMP and COMP codes. Nielsen does not provide any picture of the velocity distribution in his experiment, but for the sake of comparison figure 4.4.c shows the velocity field that Awbi [42] predicted using a $k-\epsilon$ model to represent turbulence parameters, for an identical inlet-outlet configuration, and with similar geometric characteristics and inlet airflow velocity 1.5 m/s.

In the third case for which the two codes were applied, the airflow is introduced at the top of the left side wall, with inlet flow parallel to the ceiling, and is drawn into a return placed at the bottom of the same wall. This configuration was used by Murakami et al. [25] in his model room, where he investigated the air movement. Geometric similitude requirements were satisfied by the computational domain, and the Reynolds number was 1.6×10^4 for both the numerical and experimental models. Figures 4.5.a, 4.5.b, and 4.5.c show the experimental and the predicted velocity fields as determined by Murakami et al. [25], the INCOMP, and the COMP code respectively. Also in figure 4.5.d, the distribution of the velocity vectors is given, as it was obtained by Murakami using the $k-\epsilon$ model.

Numerical simulations by the two codes developed in the current work, were

also performed for modified inlet-outlet configurations. Figures 4.6.a, 4.6.b and 4.7.a, 4.7.b present the predicted airflows for a common case in ventilation systems, where the air supply terminals are located on the one end of the ceiling, and the outlet is placed either on the other end of it or low on the opposite wall. The inlet velocity is 3 m/s, resulting in a Reynolds number of 7.7×10^4 . Figures 4.8.a, 4.8.b, and 4.8.c, show the velocity distributions obtained by the INCOMP code, while using the geometry and Reynolds number specified in Nielsen's experiment, and varying the inlet-outlet configurations. Finally, figure 4.9 shows the numerical prediction of the INCOMP code, for the geometry of the first case, modified by moving the inlet slot towards the center of the wall.

By inspecting the numerical predictions of the INCOMP code in comparison with the experimental data, it is clear that the general trend of the airflows is correctly reproduced. Although discrepancies occur, particularly in the region close to the ceiling and the floor, the numerical and experimental results are in agreement. The errors observed near the walls do not affect the accuracy of predicting the area of reverse flow. Furthermore, the INCOMP code was able to predict correctly some known characteristics of the airflows in ventilated rooms. The extensive recirculating zones which are experienced in ventilation work are represented satisfactorily. Comparison of the velocity fields shown in figures 4.4.a, 4.8.a, 4.8.b, 4.8.c leads to the conclusion that the location of the exhaust opening in a room—in contrast to the supply system—has very small influence on the entire flow field. This is a widely accepted principle in ventilation systems and has been noticed in several experimental studies [2, 45, 51]. Also figures 4.9 and 4.1.a reveal the relation of the attachment length to the distance of the bottom of the inlet slot from the floor, in accordance with the experimental flow visualizations by Timmons et al. [13, 14]. Finally, figure 4.9 shows the development of a secondary recirculatory eddy at the left top of the room, in agreement with experimental observations by Zhang et al. [5].

However, in all the numerical simulations of the INCOMP code, the inflow jet reaches the opposite wall, is deflected and then flows down along the wall, while the air velocity is maintained high. In reality, an interference to the flow is expected in

larger distances from the wall opposite the diffuser. Consequently, the code fails to predict the decay of a wall jet, mainly due to the absence of diffusive terms. Since the position of the flow inlet relative to the computational grid does not give rise to any false diffusion, and considering the assumptions of the code, it is apparent that the predicted recirculatory flows result from pressure gradients which exhibit a two-way space behaviour. Once the pressure gradients establish a recirculatory zone, there is no viscosity effect present to limit it, and as a result, the recirculatory zones occupy the whole space in a room. A careful analysis of the experimental data used for comparison, shows that the Reynolds number is in the range of 1.0×10^4 – 2.0×10^4 for all the cases. It is believed that at this range of Reynolds numbers, the turbulence present is sufficient to develop the large recirculatory zones which are observed. In the author's opinion, the good agreement obtained from the numerical simulations —considering the simplicity of the code— is due to the relatively small effect of viscous forces in the airflow pattern, in the range of Reynolds numbers where the experiments were conducted, except perhaps near solid boundaries. Therefore, the applicability of the INCOMP code for a broad range of Reynolds numbers, is questionable. It is strongly suspected that for low Reynolds number flows (less than 1.0×10^4), the predicted velocity values will deviate more and more from the real ones. However, as discussed in Chapter 1, this is a general problem encountered also in much more sophisticated ventilation computer codes.

Contrary to the INCOMP code, the calculations performed by the COMP code did not yield any comparable results. The COMP code fails to reproduce the airflow pattern in all the test cases presented. Very small velocities appear in large areas of the flow field. Upon comparing the numerical results obtained by the COMP code with the available experimental data, it is concluded that the flow field solution has been smeared, and the features of the flow have been lost. This phenomenon is believed to be caused by the following factors.

Firstly, the diffusive damping coefficients, which are implemented in the code to overcome instabilities, though small, inhibit the pressure gradients from developing and forming recirculation zones. Additionally, the fact that when solving for the

half-time, half-space step fluid properties, an average value of the neighboring node points is used; which also introduces a smearing effect.

The excessive smoothness of the flow field, leads to the hypothesis that apart from the diffusive damping influence, there is also a numerical viscosity effect on the flow configuration. Indeed, Roache [52] proved that for nonunity Courant number, and for fixed outflow boundary, there is an inherent artificial viscosity in the two-step Lax-Wendroff methods. The artificial viscous term introduced, is spatially varying, and is equal to $u^3 \frac{\Delta t}{2}$ and $v^3 \frac{\Delta t}{2}$ for the x and y directions respectively. Since the Courant number cannot be unity for all the grid points, this numerical viscosity is present in the COMP code.

Finally, the round-off errors have a disproportionate effect in the case of the compressible approach. Since the observed density variations in the computational domain are up to 0.1%, and the density gradients play a crucial role in determining the pressure field, with such small density differences the pressure gradients cannot be resolved to the required accuracy, even if double precision resolution is used. A demonstration of this feature, which arises when flows of very low Mach number are treated as compressible, has been given by Issa [8].

4.2 Partitioned ventilated rooms

The final aim of this research is to simulate the ventilation air penetration in an office complex where partitions are present. For this purpose, numerical experiments were conducted by both codes, for an office geometry subdivided into two and three workstations, by one and two partitions respectively. The supply air is introduced vertically downward and exhausts at the top right corner. Different cases were considered by simulating various configurations of the partition(s). For each variation considered, the effect on the airflow circulation in a workstation was qualified, by calculating the total volume flow rate that crosses the control surface. The control volume of a workstation is enclosed by the control surfaces consisting of the walls or partitions on the sides, the floor on the bottom, and a plane across the lowest top of the partition(s), unless otherwise stated. Comparisons

were made between numerical results obtained from the same code. At this point, it should be stated that the author is not aware of any available experimental data to compare with for the case of workstations separated by partitions.

4.2.1 Single partitioned room

The first geometry examined was the airflow in a 2.4m high by 3.2m long section, with a partition placed almost midway between the supply air inlet and the exhaust outlet, thus defining two workstations. The first condition that was studied, was for a 1.4m high partition, set with its base on the floor. Figure 4.10.a shows the velocity vector plot for this case (case 'a') obtained by the INCOMP code. Variations of this case, obtained by the same code, are shown in figures 4.10.b, 4.10.c, 4.10.d, and 4.10.e. In figure 4.10.b, the top of the partition was maintained, but 0.3m were removed from the bottom, to allow air to flow under the partition (case 'b'). Figure 4.10.c shows the same geometry of case 'a', but the partition has now a thickness of 0.2m (case 'c'). In figure 4.10.d, the bottom of the partition is on the floor, but its top is only 0.8m from it (case 'd'). Finally, in figure 4.10.e the air penetration is simulated for the case of a thick (0.8m) obstacle, 1m high (case 'e').

As a measure of comparison for the air circulation through the workstations, the unit volume flow rate was calculated for each case, based on the total volume flow rate crossing the control surfaces enclosing the workstations. The top boundary of the control volume was set at 1.4m. Comparison of the unit volume flow rates between cases 'a' and 'b' shows that a 14% decrease in the air circulation for the first workstation, and a 40% decrease for the second one results when the bottom of the partition is on the floor. A thin partition does not affect the unit volume flow rate for either of the workstations, but a thick obstacle (case 'e') will significantly decrease the air circulation in the second workstation. Increasing the height of the partition (which extends to the floor) affects the air circulation in the second workstation considerably (64% less air circulation in case 'c' compared with case 'd') and to a smaller extent in the first workstation (18% less in case 'c').

Apart from the adequacy of air flow circulation for each case, another criterion —of equal importance— for successful ventilation, is the magnitude of the maximum velocity that appears in the workstations. High velocity regions of the flow in the occupied zone are undesirable and result in uncomfortable draughts. From this point of view, the cutting out of the bottom of the partition produces unwanted large velocities, and therefore should be avoided unless the overall flow rate is reduced to reduce draughts. Moreover, although the overall air circulation in the second workstation is satisfactory, the velocity vector plot reveals that a rather large area near the partition is not ventilated properly (case 'b').

Numerical studies for a double workstation, were also performed by the COMP code. When a 1.4m high partition, set with its base on the floor (figure 4.11.a) was raised 0.4m from the floor, so that the top is now 1.8m from the floor (figure 4.11.b), the air circulation in the first workstation was almost double what it had been with the partition resting on the floor, while in the second workstation the rise is even more dramatic. It should be observed that there is only very small air circulation when the partition is on the floor. Similar increase in air circulation is detected, when a thick obstacle, 1.4m high, with its bottom cut (figure 4.11.c), is elevated until it becomes a ceiling mounted obstacle (figure 4.11.d).

4.2.2 Double partitioned room

The numerical experiments described in the previous subsection for two workstations, were repeated for a group of three workstations. The overall office area is 9m long and 2.6m high, and two partitions separate it into three equal spaces. Again, in order to carry out quantitative comparisons, the unit volume flow rate was calculated for every workstation, in each case. Figures 4.12.a, 4.12.b, 4.12.c show the velocity vector plots obtained by the INCOMP code for the case where both the 1.4m high partitions are set on the floor (case 'a'), the case where 0.4m is cut from the bottom of the left partition (case 'b'), and the case where 0.4m is cut from the bottom of both partitions (case 'c').

The velocity vector representation of the airflows, displays the domination of

each workstation by recirculating zones. When the bottom part of a partition is cut, an opposite circulation vortex is produced, and the centre of the recirculation moves upwards. Uncomfortable high velocities appear between the floor and the bottom of the partition, while at the upper part of the office, near the ceiling, two opposite flow streams are encountered, resulting in low velocities. When the bottom of one or two partitions is removed, the centre and right workstations are affected. The air circulation in the centre workstation is 74% less in case 'a' when compared with case 'b', and 69% less when compared with case 'c'. Similarly, the air circulation at the right workstation is 43% less in case 'a' compared with case 'b' and 79% less when compared with case 'c'. Finally, when only the left partition is cut (case 'b'), there is a 19% increase in the air circulation through the centre workstation when compared with case 'c', but the one at the right experiences a 64% decrease.

Numerical studies for the case of three workstations were also performed by the COMP code. Figure 4.13.a shows the velocity vector plot when the two partitions are extending to the floor (case 'd'). Raising the left partition 0.4m from the floor (figure 4.13.b, case 'e') produces a 47% increase in the circulation at the centre workstation. Raising both partitions (figure 4.13.c, case 'f') resulted in a 52% and 29% increase in the air circulation through the centre and right workstation respectively. A variation of the last case was considered by removing 0.4m from the bottom of the partitions (figure 4.13.d), instead of elevating them. When compared with case 'd', it presents a 46% increase in the air circulation in the centre workstation, and a 26% increase for the one at the exhaust end. When compared with case 'f', it shows a 10% decrease in the air circulation through the centre workstation, and a 3% decrease for the right one.

Chapter 5

Conclusions and Recommendations

The primary objective of this thesis was to develop a computer code capable of predicting the airflow of ventilated spaces. For this purpose, a compressible and incompressible approach were pursued and two codes, the COMP and the INCOMP, were developed for each, respectively. Comparison with experimental data shows that the numerical results obtained by the INCOMP code are in agreement, and the general trend of the airflow is reproduced to satisfactory tolerance. This indicates that for the specific problem in mind, the use of sophisticated models may not be justified. Even a simple model can be used, as a preliminary test, for the efficiency of a ventilated system, at least for a limited range of inflow Reynolds numbers.

On the other hand, the results from the COMP code did not yield as useful information. It is believed that the compressible approach should be abandoned, since for low Mach number flows, the numerical and machine errors become disproportionately significant.

For future work on the development of a general computer code, that can be used as a tool to provide guide lines for the design of ventilation systems, the following recommendations are made, presented in order of priority:

1. A three-dimensional solution should be developed based on the existing INCOMP code.

2. The code should be modified to allow for the effects of viscosity. Thus, it would be applicable for a broad range of Reynolds numbers.
3. Sources of contamination, and the diffusion of such materials should be added in the code, to allow for the numerical simulation of the contamination distribution in a ventilated room.

The above modifications should be made in such a way, that the resulting code can be used as a subroutine of a larger code that would evaluate the thermal comfort conditions of an arbitrary room geometry. Finally, it is implied that each modification of the model should be tested by appropriate experimental results that would validate the predictions of the code.

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TABLES

Table 1.1: Geometric variables and flow conditions, used to specify the simulated test conditions in section 4.1

Figure Number	H (cm)	L (cm)	d_1 (cm)	d_2 (cm)	B_1 (cm)	B_2 (cm)	U_i (m/s)	Configuration style
4.1.a	200	400	20	40	40	80	1.4	I
4.1.b	200	400	20	40	40	80	1.4	I
4.4.a	280	830	15	30	265	0	1.0	I
4.4.b	280	830	15	30	265	0	1.0	I
4.4.c	280	840	30	30	280	0	1.5	I
4.5.b	150	150	15	15	135	0	1.7	II
4.5.c	150	150	15	15	135	0	1.7	II
4.6.a	240	360	40	40	240	240	3.0	III
4.6.b	240	360	40	40	240	240	3.0	III
4.7.a	240	360	40	40	240	0	3.0	IV
4.7.b	240	360	40	40	240	0	3.0	IV
4.8.a	280	830	15	30	265	280	1.0	V
4.8.b	280	830	15	30	280	280	1.0	III
4.8.c	280	830	15	30	280	0	1.0	IV
4.9	200	400	20	40	90	80	1.4	I

Inlet-outlet configuration styles

Table 1.2: Computational characteristics used to specify the simulated test conditions in section 4.1

Figure Number	Code	Mesh size Δx (cm)	Mesh size Δy (cm)	F_x	F_y	Minimum relative velocity plotted
4.1.a	INCOMP	20	20	-	-	0.1
4.1.b	COMP	10	10	0.01	0.01	0.01
4.4.a	INCOMP	15	15	-	-	0.1
4.4.b	COMP	10	10	0.01	0.01	0.01
4.5.b	INCOMP	15	15	-	-	0.1
4.5.c	COMP	5	5	0.005	0.005	0.03
4.6.a	INCOMP	20	20	-	-	0.1
4.6.b	COMP	10	10	0.005	0.005	0.1
4.7.a	INCOMP	40	40	-	-	0.1
4.7.b	COMP	20	20	0.005	0.005	0.05
4.8.a	INCOMP	15	15	-	-	0.1
4.8.b	INCOMP	15	15	-	-	0.1
4.8.c	INCOMP	15	15	-	-	0.1
4.9	INCOMP	10	10	-	-	0.1

Table 2.1: Geometric variables and flow conditions, used to specify the simulated test conditions in subsection 4.2.1

Common dimensions

L (cm)	H (cm)	d_1 (cm)	d_2 (cm)	B_1 (cm)	B_2 (cm)
320	240	40	40	240	240

Figure Number	d_3 (cm)	d_4 (cm)	h_1 (cm)	h_2 (cm)	t_1 (cm)	U_i (m/s)
4.10.a	140	180	140	0	1	5.0
4.10.b	140	180	100	30	1	5.0
4.10.c	140	160	140	0	20	5.0
4.10.d	140	160	80	0	20	5.0
4.10.e	120	120	100	0	80	5.0
4.11.a	140	160	140	0	20	5.0
4.11.b	140	160	140	40	20	5.0
4.11.c	135	135	140	40	50	5.0
4.11.d	135	135	140	100	50	5.0

Table 2.2: Computational characteristics used to specify the simulated test conditions in subsection 4.2.1

Figure Number	Code	Mesh size Δx (cm)	Mesh size Δy (cm)	F_x	F_y	Minimum relative velocity plotted
4.10.a	INCOMP	20	20	-	-	0.1
4.10.b	INCOMP	20	20	-	-	0.1
4.10.c	INCOMP	20	20	-	-	0.1
4.10.d	INCOMP	20	20	-	-	0.1
4.10.e	INCOMP	20	20	-	-	0.1
4.11.a	COMP	10	10	0.01	0.01	0.1
4.11.b	COMP	10	10	0.01	0.01	0.1
4.11.c	COMP	10	10	0.01	0.01	0.1
4.11.d	COMP	10	10	0.01	0.01	0.1

Table 3.1: Geometric variables and flow conditions, used to specify the simulated test conditions in subsection 4.2.2

Common dimensions

L (cm)	H (cm)	d_1 (cm)	d_2 (cm)	d_3 (Left part.) (cm)	d_4 (Right part.) (cm)	B_1 (cm)	B_2 (cm)	t_1 (cm)
900	260	40	40	290	290	260	260	20

Figure Number	h_1 (Left part.) (cm)	h_2 (Left part.) (cm)	h_1 (Right part.) (cm)	h_2 (Right part.) (cm)	U_i (m/s)
4.12.a	140	0	140	0	10.0
4.12.b	100	40	140	0	10.0
4.12.c	100	40	100	40	10.0
4.13.a	140	0	140	0	10.0
4.13.b	140	40	140	0	10.0
4.13.c	140	40	140	40	10.0
4.13.d	100	40	100	40	10.0

Table 3.2: Computational characteristics used to specify the simulated test conditions in subsection 4.2.2

Figure Number	Code	Mesh size Δx (cm)	Mesh size Δy (cm)	F_x	F_y	Minimum relative velocity plotted
4.10.a	INCOMP	20	20	-	-	0.05
4.10.b	INCOMP	20	20	-	-	0.05
4.10.c	INCOMP	20	20	-	-	0.05
4.10.d	COMP	10	10	0.01	0.01	0.05
4.10.e	COMP	10	10	0.01	0.01	0.05
4.11.a	COMP	10	10	0.01	0.01	0.05
4.11.b	COMP	10	10	0.01	0.01	0.05

FIGURES

Fig. 2.1 Finite difference grid for COMP code.

Fig. 2.2 Control volume for half time step point.

Fig. 2.3 Solid wall boundary for COMP code

Fig. 2.4 Corner boundary point for COMP code

Fig. 2.5.a Relationship between first and second steps for 1-D case

Fig. 2.5.b Outflow boundary for COMP code

Fig. 2.6 Grid point at the sharp convex corner

Fig. 2.7 Outline flow chart of the COMP code

Fig. 2.7 (cont.)

Fig. 2.8.a Behaviour of the compressible scheme for a simple pipe case 1.5 m long. (The time steps adopted, are with reference to the maximum allowable time step. Inlet velocity: 5m/s, mesh size $\Delta x=0.15\text{m}$)

Fig. 2.8.b Behaviour of the compressible scheme for a simple pipe case 1.5 m long. (Same conditions as for fig. 2.8.a)

Fig. 2.8.c Behaviour of the compressible scheme for a simple pipe case 1.5 m long. (The time steps adopted, are with reference to the maximum allowable time step. Inlet velocity: 15m/s, mesh size $\Delta x=0.15\text{m}$)

Fig. 2.8.d Behaviour of the compressible scheme for a simple pipe case 1.5 m long. (Same conditions as for fig. 2.8.b)

Fig. 2.9 Velocity vector plot for a corner pipe case obtained by the COMP code (inlet velocity: 5m/s, $L=3\text{m}$, $H=3\text{m}$, $d_1=1.5\text{m}$, $d_2=1.5\text{m}$. Mesh size $\Delta x = \Delta y = 0.1\text{m}$, $DT=0.6\Delta t_{\max}$, $F_x = F_y = 0.01$).

Fig. 3.1 Staggered grid arrangement for the INCOMP code.

Fig. 3.2 Notation for the u-momentum control volume analysis for section 3.1.

Fig. 3.3 Notation for the v-momentum control volume analysis for section 3.1.

Fig. 3.4 Notation for the pressure-correction equation.

Fig. 3.5 Physical domain and computational boundaries in INCOMP code.

Fig. 3.6 Specified velocity at the wall boundary in INCOMP code.

Fig. 9.7 Outline flow chart of the INCOMP code

Fig. 3.7 (cont.)

Fig. 3.8.a Velocity vector plot for a corner pipe case obtained by the INCOMP code (inlet velocity: 5m/s, $L=3.2\text{m}$, $H=1.6\text{m}$, $d_1=1.6\text{m}$, $d_2=0.8\text{m}$, mesh size $\Delta x = \Delta y = 0.4\text{m}$, exit velocity prescribed).

Fig. 3.8.b Velocity vector plot for a corner pipe case obtained by the INCOMP code (same geometric and flow conditions as for fig. 3.8.a, mesh size $\Delta x = \Delta y = 0.2\text{m}$, exit velocity prescribed).

Fig. 3.8.c Velocity vector plot for a corner pipe case obtained by the INCOMP code (same geometric and flow conditions as for fig. 3.8.a, mesh size $\Delta x = \Delta y = 0.4\text{m}$, exit pressure prescribed).

Fig. 4.1.a Velocity vectors obtained by the INCOMP code, simulating Timmons' experiment [14] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.1.b Velocity vectors obtained by the COMP code, simulating Timmons' experiment [14] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.2.a Comparison between predicted and measured [14] velocity profiles.

Fig. 4.2.b Comparison between predicted and measured [14] velocity profiles.

Fig. 4.2.c Comparison between predicted and measured [14] velocity profiles.

Fig. 4.9 Comparison between predicted and measured [3, 11] velocity profiles.

Fig. 4.4.a Velocity vectors obtained by the INCOMP code, simulating Nielsen's experiment [3, 11] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.4.b Velocity vectors obtained by the COMP code, simulating Nielsen's experiment [3, 11] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.4.c Predicted velocity vectors for isothermal mode (Awbi [42]). (see Table 1.1 for geometric and flow conditions).

Fig. 4.5.a Experimental velocity vectors (Murakami et al. [25]).

Fig. 4.5.b Velocity vectors obtained by the INCOMP code, simulating Murakami's experiment [25] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.5.c Velocity vectors obtained by the COMP code, simulating Murakami's experiment [25] (see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.5.d Velocity vectors obtained by the $k-\epsilon$ turbulence model (Murakami et al. [25]).

Fig. 4.6.a Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.6.b Velocity vectors obtained by the COMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.7.a Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.7.b Velocity vectors obtained by the COMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.8.a Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.8.b Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.8.c Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.9 Velocity vectors obtained by the INCOMP code
(see Tables 1.1 and 1.2 for simulation parameters).

Fig. 4.10.a Simulation of single partitioned case by the INCOMP code (see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.10.b Simulation of single partitioned case by the INCOMP code (see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.10.c Simulation of single partitioned case by the INCOMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.10.d Simulation of single partitioned case by the INCOMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.10.e Simulation of single partitioned case by the INCOMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.11.a Simulation of single partitioned case by the COMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.11.b Simulation of single partitioned case by the COMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.11.c Simulation of single partitioned case by the COMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.11.d Simulation of single partitioned case by the COMP code
(see Tables 2.1 and 2.2 for simulation parameters).

Fig. 4.12.a Simulation of double partitioned case by the INCOMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Resolution Test Chart Labels:

- 1.0
- 1.1
- 1.25
- 1.4
- 1.6
- 1.8
- 2.0
- 2.2
- 2.5
- 2.8
- 3.0
- 3.2
- 3.6
- 4.0

[illegible]

Fig. 4.12.b Simulation of double partitioned case by the INCOMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Fig. 4.12.c Simulation of double partitioned case by the INCOMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Fig. 4.19.a Simulation of double partitioned case by the COMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Fig. 4.19.b Simulation of double partitioned case by the COMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Fig. 4.19.c Simulation of double partitioned case by the COMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Fig. 4.19.d Simulation of double partitioned case by the COMP code
(see Tables 3.1 and 3.2 for simulation parameters).

Appendix A

Finite difference equations for the COMP code

This section contains the half-time and full-time step equations in two dimensions, for a regular rectangular cell.

A.1 Half-time step equations

Continuity equation

$$\begin{aligned}\rho_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} = & \frac{1}{4}(\rho_{i,j}^n + \rho_{i,j+1}^n + \rho_{i+1,j}^n + \rho_{i+1,j+1}^n) + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u)_{i,j}^n + (\rho u)_{i+1,j}^n - (\rho u)_{i,j+1}^n \\ & - (\rho u)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v)_{i,j}^n + (\rho v)_{i,j+1}^n - (\rho v)_{i+1,j}^n - (\rho v)_{i+1,j+1}^n]\end{aligned}$$

$$\begin{aligned}\rho_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} = & \frac{1}{4}(\rho_{i,j}^n + \rho_{i,j+1}^n + \rho_{i-1,j}^n + \rho_{i-1,j+1}^n) + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u)_{i-1,j}^n + (\rho u)_{i,j}^n - (\rho u)_{i-1,j+1}^n \\ & - (\rho u)_{i,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v)_{i-1,j}^n + (\rho v)_{i-1,j+1}^n - (\rho v)_{i,j}^n - (\rho v)_{i,j+1}^n]\end{aligned}$$

$$\begin{aligned}\rho_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} = & \frac{1}{4}(\rho_{i,j-1}^n + \rho_{i,j}^n + \rho_{i+1,j-1}^n + \rho_{i+1,j}^n) + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u)_{i,j-1}^n + (\rho u)_{i+1,j-1}^n - (\rho u)_{i,j}^n \\ & - (\rho u)_{i+1,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v)_{i,j-1}^n + (\rho v)_{i,j}^n - (\rho v)_{i+1,j-1}^n - (\rho v)_{i+1,j}^n]\end{aligned}$$

$$\begin{aligned}\rho_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}(\rho_{i-1,j-1}^n + \rho_{i-1,j}^n + \rho_{i,j-1}^n + \rho_{i,j}^n) + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u)_{i-1,j-1}^n + (\rho u)_{i,j-1}^n - (\rho u)_{i-1,j}^n \\ &\quad - (\rho u)_{i,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v)_{i-1,j-1}^n + (\rho v)_{i-1,j}^n - (\rho v)_{i,j-1}^n - (\rho v)_{i,j}^n]\end{aligned}$$

X-Momentum equation

$$\begin{aligned}(\rho u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho u)_{i,j}^n + (\rho u)_{i,j+1}^n + (\rho u)_{i+1,j}^n + (\rho u)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u^2 + P)_{i,j}^n \\ &\quad + (\rho u^2 + P)_{i+1,j}^n - (\rho u^2 + P)_{i,j+1}^n - (\rho u^2 + P)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho uv)_{i,j}^n \\ &\quad + (\rho uv)_{i,j+1}^n - (\rho uv)_{i+1,j}^n - (\rho uv)_{i+1,j+1}^n]\end{aligned}$$

$$\begin{aligned}(\rho u)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho u)_{i,j}^n + (\rho u)_{i,j+1}^n + (\rho u)_{i-1,j}^n + (\rho u)_{i-1,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u^2 + P)_{i-1,j}^n \\ &\quad + (\rho u^2 + P)_{i,j}^n - (\rho u^2 + P)_{i-1,j+1}^n - (\rho u^2 + P)_{i,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho uv)_{i-1,j}^n \\ &\quad + (\rho uv)_{i-1,j+1}^n - (\rho uv)_{i,j}^n - (\rho uv)_{i,j+1}^n]\end{aligned}$$

$$\begin{aligned}(\rho u)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho u)_{i,j-1}^n + (\rho u)_{i,j}^n + (\rho u)_{i+1,j-1}^n + (\rho u)_{i+1,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u^2 + P)_{i,j-1}^n \\ &\quad + (\rho u^2 + P)_{i+1,j-1}^n - (\rho u^2 + P)_{i,j}^n - (\rho u^2 + P)_{i+1,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho uv)_{i,j-1}^n \\ &\quad + (\rho uv)_{i,j}^n - (\rho uv)_{i+1,j-1}^n - (\rho uv)_{i+1,j}^n]\end{aligned}$$

$$\begin{aligned}(\rho u)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho u)_{i-1,j-1}^n + (\rho u)_{i-1,j}^n + (\rho u)_{i,j-1}^n + (\rho u)_{i,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho u^2 + P)_{i-1,j-1}^n \\ &\quad + (\rho u^2 + P)_{i,j-1}^n - (\rho u^2 + P)_{i-1,j}^n - (\rho u^2 + P)_{i,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho uv)_{i-1,j-1}^n \\ &\quad + (\rho uv)_{i-1,j}^n - (\rho uv)_{i,j-1}^n - (\rho uv)_{i,j}^n]\end{aligned}$$

Y-Momentum equation

$$\begin{aligned}
 (\rho v)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho v)_{i,j}^n + (\rho v)_{i,j+1}^n + (\rho v)_{i+1,j}^n + (\rho v)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v^2 + P)_{i,j}^n \\
 &+ (\rho v^2 + P)_{i,j+1}^n - (\rho v^2 + P)_{i+1,j}^n - (\rho v^2 + P)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho v u)_{i,j}^n \\
 &+ (\rho v u)_{i+1,j}^n - (\rho v u)_{i,j+1}^n - (\rho v u)_{i+1,j+1}^n]
 \end{aligned}$$

$$\begin{aligned}
 (\rho v)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho v)_{i,j}^n + (\rho v)_{i,j+1}^n + (\rho v)_{i-1,j}^n + (\rho v)_{i-1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v^2 + P)_{i-1,j}^n \\
 &+ (\rho v^2 + P)_{i-1,j+1}^n - (\rho v^2 + P)_{i,j}^n - (\rho v^2 + P)_{i,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho v u)_{i-1,j}^n \\
 &+ (\rho v u)_{i,j}^n - (\rho v u)_{i-1,j+1}^n - (\rho v u)_{i,j+1}^n]
 \end{aligned}$$

$$\begin{aligned}
 (\rho v)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho v)_{i,j-1}^n + (\rho v)_{i,j}^n + (\rho v)_{i+1,j-1}^n + (\rho v)_{i+1,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v^2 + P)_{i,j-1}^n \\
 &+ (\rho v^2 + P)_{i,j}^n - (\rho v^2 + P)_{i+1,j-1}^n - (\rho v^2 + P)_{i+1,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho v u)_{i,j-1}^n \\
 &+ (\rho v u)_{i+1,j-1}^n - (\rho v u)_{i,j}^n - (\rho v u)_{i+1,j}^n]
 \end{aligned}$$

$$\begin{aligned}
 (\rho v)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho v)_{i-1,j-1}^n + (\rho v)_{i-1,j}^n + (\rho v)_{i,j-1}^n + (\rho v)_{i,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4}[(\rho v^2 + P)_{i-1,j-1}^n \\
 &+ (\rho v^2 + P)_{i-1,j}^n - (\rho v^2 + P)_{i,j-1}^n - (\rho v^2 + P)_{i,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho v u)_{i-1,j-1}^n \\
 &+ (\rho v u)_{i,j-1}^n - (\rho v u)_{i-1,j}^n - (\rho v u)_{i,j}^n]
 \end{aligned}$$

Energy equation

$$\begin{aligned}
 (\rho e)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho e)_{i,j}^n + (\rho e)_{i,j+1}^n + (\rho e)_{i+1,j}^n + (\rho e)_{i+1,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4}[(\rho e + P)u]_{i,j}^n \\
 &+ [(\rho e + P)u]_{i+1,j}^n - [(\rho e + P)u]_{i,j+1}^n - [(\rho e + P)u]_{i+1,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4} \\
 &[[(\rho e + P)v]_{i,j}^n + [(\rho e + P)v]_{i,j+1}^n - [(\rho e + P)v]_{i+1,j}^n - [(\rho e + P)v]_{i+1,j+1}^n]
 \end{aligned}$$

$$\begin{aligned}
(\rho e)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho e)_{i,j}^n + (\rho e)_{i,j+1}^n + (\rho e)_{i-1,j}^n + (\rho e)_{i-1,j+1}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4} [(\rho e + P)u]_{i-1,j}^n \\
&+ [(\rho e + P)u]_{i,j}^n - [(\rho e + P)u]_{i-1,j+1}^n - (\rho e + P)u]_{i,j+1}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4} \\
&[[(\rho e + P)v]_{i-1,j}^n + [(\rho e + P)v]_{i-1,j+1}^n - [(\rho e + P)v]_{i,j}^n - [(\rho e + P)v]_{i,j+1}^n]
\end{aligned}$$

$$\begin{aligned}
(\rho e)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho e)_{i,j-1}^n + (\rho e)_{i,j}^n + (\rho e)_{i+1,j-1}^n + (\rho e)_{i+1,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4} [(\rho e + P)u]_{i,j-1}^n \\
&+ [(\rho e + P)u]_{i+1,j-1}^n - [(\rho e + P)u]_{i,j}^n - (\rho e + P)u]_{i+1,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4} \\
&[[(\rho e + P)v]_{i,j-1}^n + [(\rho e + P)v]_{i,j}^n - [(\rho e + P)v]_{i+1,j-1}^n - [(\rho e + P)v]_{i+1,j}^n]
\end{aligned}$$

$$\begin{aligned}
(\rho e)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} &= \frac{1}{4}[(\rho e)_{i-1,j-1}^n + (\rho e)_{i-1,j}^n + (\rho e)_{i,j-1}^n + (\rho e)_{i,j}^n] + \frac{\Delta t}{\Delta x} \frac{1}{4} [(\rho e + P)u]_{i-1,j-1}^n \\
&+ [(\rho e + P)u]_{i,j-1}^n - [(\rho e + P)u]_{i-1,j}^n - (\rho e + P)u]_{i,j}^n] + \frac{\Delta t}{\Delta y} \frac{1}{4} \\
&[[(\rho e + P)v]_{i-1,j-1}^n + [(\rho e + P)v]_{i-1,j}^n - [(\rho e + P)v]_{i,j-1}^n - [(\rho e + P)v]_{i,j}^n]
\end{aligned}$$

A.2 Full-time step equations

Continuity equation

$$\begin{aligned}
\rho_{i,j}^{n+1} &= \rho_{i,j}^n + \frac{\Delta t}{\Delta x} \frac{1}{2} [(\rho u)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho u)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho u)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} \\
&- (\rho u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] + \frac{\Delta t}{\Delta y} \frac{1}{2} [(\rho v)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho v)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}]
\end{aligned}$$

X-Momentum equation

$$\begin{aligned}
(\rho u)_{i,j}^{n+1} &= (\rho u)_{i,j}^n + \frac{\Delta t}{\Delta x} \frac{1}{2} [(\rho u^2 + P)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho u^2 + P)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho u^2 + P)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} \\
&- (\rho u^2 + P)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] + \frac{\Delta t}{\Delta y} \frac{1}{2} [(\rho uv)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho uv)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} \\
&- (\rho uv)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - (\rho uv)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}]
\end{aligned}$$

Y-Momentum equation

$$\begin{aligned}
 (\rho v)_{i,j}^{n+1} = & (\rho v)_{i,j}^n + \frac{\Delta t}{\Delta y} \frac{1}{2} [(\rho v^2 + P)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho v^2 + P)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v^2 + P)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \\
 & - (\rho v^2 + P)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] + \frac{\Delta t}{\Delta x} \frac{1}{2} [(\rho v u)_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + (\rho v u)_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \\
 & - (\rho v u)_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - (\rho v u)_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}]
 \end{aligned}$$

Energy equation

$$\begin{aligned}
 (\rho e)_{i,j}^{n+1} = & (\rho e)_{i,j}^n + \frac{\Delta t}{\Delta x} \frac{1}{2} [(\rho e + P)u]_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} + [(\rho e + P)u]_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \\
 & - [(\rho e + P)u]_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - [(\rho e + P)u]_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}] + \frac{\Delta t}{\Delta y} \frac{1}{2} [(\rho e + P)v]_{i-\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} \\
 & + [(\rho e + P)v]_{i-\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - [(\rho e + P)v]_{i+\frac{1}{2},j-\frac{1}{2}}^{n+\frac{1}{2}} - [(\rho e + P)v]_{i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}}]
 \end{aligned}$$

END

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