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AN APPROACH TO THE SIMULATION OF COUPLED HEAT AND
MASS FLOWS IN BUILDINGS

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SYNOPSIS
This paper describes the techniques used within the ESP system to represent and solve the heat and mass conservation equations relating to combined building and plant systems. In particular, it describes the equation-sets used to represent inter-zonal (building) and inter-component (plant) fluid flow and the method used for the integration of the non-linear heat and mass flow equations. By means of a case study, the application in a real design context is demonstrated.

1 INTRODUCTION

In building systems, and the HVAC plant which services them, fluid flow phenomena are encountered in four principle areas:

- air flow through cracks and various openings in the building envelope and interior partitions in the form of infiltration and natural ventilation;
- the flow of air through the distribution networks which exist to satisfy the heating/cooling demands and ventilation requirements;
- the flow of heating/cooling fluids through the plant system network;
- and the convective fluid flows within interior building spaces and plant components.

In building design, some knowledge of the magnitude of these flows is a necessary prerequisite of load and energy calculations, system control analysis, thermal comfort assessment and contaminant/moisture dispersal estimation. Although fluid flow is demonstrably an important aspect of building/plant performance assessment, the sophistication of its treatment in many modelling systems has tended to lag the treatment applied to the other important flow paths such as the shortwave and longwave processes and conduction. The principal reason for this would appear to be the inherent computational difficulties and the uncertainty associated with the estimation of the parameters of air flow problems.

In recent times more emphasis has been placed on fluid flow simulation with two approaches extant:

Computational Fluid Dynamics (CFD)
A method in which the conservation equations for mass, momentum and thermal energy are solved for all nodal points of a two- or three-dimensional grid inside or around the object under investigation. A well known example of a CFD model is PHOENICS (Spalding 1981). While in theory the CFD approach is applicable to any thermo-fluid phenomenon, in practice, and in the building physics domain in particular, there are a several problematic issues of which the amount of necessary computing power (Chen 1988), the nature of the flow fields and the assessment of the complex, occupant-dependent boundary conditions are the most problematic. This has often led to CFD applications being restricted to the steady-state case which, in many building performance contexts, is atypical. Application examples in the field of building energy simulation are the prediction of temperature and velocity fields inside large or technically complex enclosures such as atria and television studios (Markatos 1984) and the prediction of the pressure field around a building (Haggkvist et al 1989).

The Zonal Method
A method in which a building and its plant are treated as a collection of nodes representing rooms, parts of rooms and plant components, with inter-nodal connections representing the distributed flow paths associated with cracks, doors, ducts and the like. The assumption is made that there is a simple, non-linear relationship between the flow through a connection and the pressure difference across it. Conservation of mass for the flows into and out of each node leads to a set of simultaneous, non-linear equations which can be integrated over time to characterise the flow domain.

In the context of combined heat and mass flow simulation it is the zonal method which has proved (for the present at least) to be most commensurate with the modelling approach adopted.
by the ESP system. The reasons for this are threefold. Firstly, the number of nodes involved - say some 100-200 in a moderately sized building - is considerably less than employed in a CFD approach and so the additional CPU burden is acceptable. Secondly, there is a strong relationship between the nodal networks which represent the fluid regime and the thermal counterpart. This means that the information demands of the energy balance formulations can be directly satisfied. And, finally, the technique can be readily applied to combined multi-zone buildings and multi-component, multi-network plant systems.

It is the zonal method then which has been employed for several years as the basis of the air flow element of the ESP system and which underpins recent developments which have led to an improved equation solver and extensions of the technique to plant systems in general. Within ESP these developments are made available to a user via ESPmfs for use in cases where buoyancy effects are time-invariant, and as an integral encapsulation within ESPbps, the main simulation module, for use in cases where buoyancy has a strong temporal dimension.

This paper describes the theoretical basis of the ESP approach to fluid flow simulation in terms of the flow equation types offered and the underlying numerical solution strategy. The integration of the algorithm within the ESPbps numerical processing scheme is then described to demonstrate the technique employed to achieve combined heat and fluid flow in building/plant systems. Finally, and briefly, the paper illustrates the application of the approach in practice.

2 THE APPROACH IN OUTLINE

Within the ESP approach, during each simulation time step, the problem is constrained to the steady flow (possibly bi-directional) of an incompressible fluid along the connections which represent the building/plant mass flow network when subjected to certain boundary conditions regarding pressure and/or flow. The problem reduces therefore to the calculation of fluid flow through these connections with the nodes of the network representing either internal or boundary pressures. This is achieved by an iterative mass balance approach in which nodal pressures are adjusted until the mass residual of each internal node satisfies some user-specified criterion. However, all nodes and components within a sub-network must relate to the same fluid type.

Information on potential mass flows is given by a user in terms of node descriptions, fluid types, flow component types, interconnections and boundary conditions. In this way a nodal network (or perhaps several decoupled sub-networks) of connecting resistances is constructed. This may then be attached, at its boundaries, to known pressures or to pressure coefficient sets which represent the relationship between free-stream wind vectors and the building external surface pressures to result.

Nodes may represent rooms, parts of rooms, plant components, connection points in a duct or in a pipe, ambient conditions and so on. Fluid flow components correspond to discrete fluid flow passages such as doorways, construction cracks, ducts, pipes, fans, pumps, etc. As an example Figure 1 shows a sketch of a part of a building consisting of two rooms, some connections between the rooms, a radiator heating system connected to one zone and an air heating system connected to the other zone. In this case the building and plant configuration contains at least two mass flow networks - one for the air and one for the water. One possibility with respect to the translation of this configuration into a nodal scheme is indicated by the dots.

2.1 Node Definition

Nodes are characterised by several data items including an identifier, the fluid type, the node type, the height above some arbitrary datum, temperature (for use only in ESPmfs) and several supplementary parameters dependent on the node type (see later). At the present time only two
fluid types are supported - air and water - although additional types will be developed as required. The nodal types currently on offer are summarized in Table 1.

<table>
<thead>
<tr>
<th>Type</th>
<th>Supplementary data</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Internal; unknown pressure None</td>
</tr>
<tr>
<td>1</td>
<td>Internal; known pressure total pressure (Pa)</td>
</tr>
<tr>
<td>2</td>
<td>Boundary; known pressure 1) total pressure (Pa)</td>
</tr>
<tr>
<td></td>
<td>2) node temperature flag, indicating</td>
</tr>
<tr>
<td></td>
<td>0: temperature is some constant</td>
</tr>
<tr>
<td></td>
<td>1: temperature equals outside air temperature</td>
</tr>
<tr>
<td>3</td>
<td>Boundary; wind pressure + 1) wind pressure coefficients index</td>
</tr>
<tr>
<td></td>
<td>temperature = outside air 2) surface azimuth (* clockwise from North)</td>
</tr>
</tbody>
</table>

Table 1 Mass flow network node types

The nodes of the network represent either internal or boundary pressures. The difference is that only internal nodes are subjected to the mass balance tracking. Note that in the present context 'internal' is not necessary equivalent to 'inside' nor does 'boundary' necessarily equate to 'outside'. Usually the pressure at an internal node is unknown, although it can be treated as a known parameter as would be required, for example, in the case of an expansion vessel in a hydronic radiator system. An interesting possibility is that this node type can be used in an air infiltration problem to mimic a pressurization test, in order to compare the overall leakage characteristic with measurements.

2.1.1 Wind Induced Pressures

Pressures at boundary nodes can be specified or they can be declared to be wind induced. In the latter case a reference is made to an appropriate pressure coefficient set as held in ESP's pressure coefficients database. At run-time the pressure coefficient, appropriate to the prevailing wind direction, is used to generate the surface pressure due to the wind:

$$P_i = C_{p,i,d} \frac{1}{2} \rho V_{rd}^2 \; (Pa)$$

where $C_{p,i,d}$ is the pressure coefficient for a surface location $i$ corresponding to wind from direction $d$, $\rho$ is the air density ($kgm^{-3}$) and $V_{rd}$ is the local wind speed ($m s^{-1}$) from direction $d$ at some reference level $r$ (usually equal to the building height). The ratio between the local wind speed and the wind speed as read from the climate file, is termed the wind speed reduction.
factor. This reduction factor accounts for any difference between measurement height and building height and for intervening terrain roughness. Besides direct numerical input, ESP offers several user selectable wind profiles for evaluation of the wind speed reduction factor:

- power law wind profile (AIVC 1986):
  \[ \frac{U_l}{U_{10}} = K \left( \frac{z_m}{z_{10}} \right)^a \]  
  \[ (-) \]
  where \( U_l \) is the local wind speed at a height \( z_l \) m above the ground (ms\(^{-1}\)), \( U_{10} \) is the wind speed measured in open countryside (ms\(^{-1}\)) at a standard height of 10 m and \( K, a \) are terrain dependent constants (see Table 2)

- logarithmic wind profile (Simiu & Scanlan 1986):
  \[ \frac{U_l}{U_m} = \frac{U_{*, l}}{U_{*, m}} \left( \frac{z_{10} - d}{z_{10} - d_m} \right)^{0.1} \]  
  \[ (-) \]
  where \( U_m \) is the wind speed measured at the meteo site (ms\(^{-1}\)) at a height of \( z_m \) m above the ground, \( U_* \) is the atmospheric friction speed (ms\(^{-1}\)), \( z_0 \) is the terrain dependent roughness length (m) and \( d \) is the terrain dependent displacement length (m) (see Table 2)

- Lawrence Berkeley Laboratory (LBL) model wind profile (AIVC 1986):
  \[ \frac{U_l}{U_m} = \frac{\alpha_l (z_l/10)^{\gamma}}{\alpha_m (z_m/10)^{\gamma_m}} \]  
  \[ (-) \]
  where \( \alpha, \gamma \) are terrain dependent constants (see Table 2).

<table>
<thead>
<tr>
<th>Terrain</th>
<th>( K )</th>
<th>( a )</th>
<th>( z_0 )</th>
<th>( d )</th>
<th>( \alpha )</th>
<th>( \gamma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open flat country</td>
<td>0.68</td>
<td>0.17</td>
<td>0.03</td>
<td>0.0</td>
<td>1.00</td>
<td>0.15</td>
</tr>
<tr>
<td>Country with scattered wind breaks</td>
<td>0.52</td>
<td>0.20</td>
<td>0.1</td>
<td>0.0</td>
<td>0.85</td>
<td>0.20</td>
</tr>
<tr>
<td>Rural</td>
<td>0.35</td>
<td>0.25</td>
<td>0.5</td>
<td>0.7 h</td>
<td>0.67</td>
<td>0.25</td>
</tr>
<tr>
<td>Urban</td>
<td>0.21</td>
<td>0.33</td>
<td>&gt; 2.0</td>
<td>0.8 h</td>
<td>0.47</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Table 2 Typical values terrain dependent parameters (h = building height)

Compared with both the power law profile and the LBL wind profile, the logarithmic wind profile is to be preferred because it is based on physical laws rather than on an empirical formulation. It should be noted however that all the wind profiles above are actually only valid for heights over \((20 \times z_0 + d)\) and lower than \(60 \ldots 100 \) m. The layer below \((20 \times z_0 + d)\) is often referred to as the urban canopy. Here the wind speed and direction is strongly influenced by individual obstacles and can only be predicted through wind tunnel experiments or simulations undertaken by a CFD model. If these are not available, great care must be taken although, depending on the problem on hand, a high or low estimate of the wind speed reduction factor may be made to characterise the problem. For example, in the case of an energy consumption and infiltration problem it is safer to use a high estimate of the wind speed reduction factor (for example wind speed evaluated at a height of \((20 \times z_0 + d)\)). Alternatively, in the case of an air quality or overheating and ventilation problem it is probably safer to use a low estimate (for example wind speed evaluated at the actual building height).

To give a numerical example: assume a building with a height of 7.5 m located in an urban area (say \( z_0 = 1.0 \) m and \( d = 6 \) m ; ie. urban canopy thickness \( \approx 26 \) m), and that the wind speed was measured at a height of 10 m in an open flat country. Then the following local wind speed reduction factors at building height will result:

- power law: \( 0.58 \)
logarithmic law: 0.10 ... 0.73 (-) lower/upper estimate as indicated above
LBL profile: 0.62 (-)

2.1.2 Stack Effect

Within ESP each node is assigned a reference height. The reference height defines the mean height of the associated building zone or plant component. The node reference height may be expressed relative to any arbitrary datum level as long as this datum level is the same for all nodes in the network. The reference height is then used in the calculation of buoyancy driven flows (stack effect) in a manner similar to the approach suggested by Walton (1988).

Figure 2 An example two zone connected system

Consider Figure 2 which shows two zones connected by some fluid flow component. It is assumed that each volume can be characterised by a single temperature and a single static pressure at some height relative to a common data plane. The inlet and outlet of the connecting component are at different heights relative to each other and relative to the nodes representing the volumes. Analysis of the fluid flow through a component $i$ is based on Bernoulli’s equation for one-dimensional steady flow of an incompressible Newtonian fluid including a loss term:

$$
\Delta P_i = (\rho_1 + \rho V_1^2/2) - (\rho_2 + \rho V_2^2/2) + \rho g (z_1 - z_2) \quad (Pa)
$$

where $\Delta P_i$ is the sum of all friction and dynamic losses (Pa), $\rho_1, \rho_2$ are entry and exit static pressures (Pa), $V_1, V_2$ are entry and exit velocities $(ms^{-1})$, $\rho$ is the density of the fluid flowing through the component $(kgm^{-3})$, $g$ is the acceleration of gravity $(ms^{-2})$ and $z_1, z_2$ are the entry and exit elevations $(m)$. This equation defines a sign convention for the direction of flow: positive from point 1 to point 2 (or $n$ to $m$).

Equation 6 can be simplified by combining related terms. Dynamic pressures are the $\rho V^2/2$ terms, and total pressure is defined to be the sum of static pressure and dynamic pressure - that is $P = p + \rho V^2/2$. If nodes $n$ and $m$ represent large volumes (for example a room), the dynamic pressures are effectively zero. If the nodes represent some point in a duct or pipe network, there will be a positive dynamic pressure. The pressures at the inlet and outlet of the flow component can be related to the node pressures by the hydrostatic law:

$$
P_1 = P_n + \rho_n g (z_n - z_1) = P_n - \rho_n g h_1 \quad (Pa) \quad \text{where } h_1 = z_1 - z_n \quad (m)
$$

$$
P_2 = P_m + \rho_m g (z_m - z_2) = P_m - \rho_m g h_2 \quad (Pa) \quad \text{where } h_2 = z_2 - z_m \quad (m)
$$

The relative heights, $h_1$ and $h_2$, are a convenient way of expressing the flow component inlet and outlet heights. For example, it is quite common for flow components in the building fabric to only differ with respect to inlet and outlet heights relative to the zone heights. On the other hand, if the flow component is part of a duct or pipe network, the relative heights will be zero. Equation 6 can thus be reduced to:
\[ \Delta P_i = P_n - P_m + \rho g (z_n + h_1 - z_m - h_2) - \rho_n g h_1 + \rho_m g h_2 \ (Pa) \]  

The terms \([\rho g (z_n + h_1 - z_m - h_2) - \rho_n g h_1 + \rho_m g h_2]\) can be collectively called the stack pressure, \(PS_i\), acting on component \(i\):

\[ \begin{align*}
PS_i &= \rho_n g (z_n - z_m) + h_2 g (\rho_m - \rho_n) \ (Pa) \quad \text{(flow in positive direction)} \\
PS_i &= \rho_m g (z_n - z_m) + h_1 g (\rho_m - \rho_n) \ (Pa) \quad \text{(flow in negative direction)}
\end{align*} \]

### 2.2 Components Definition

A flow component is characterised by an identifier, a type code (indicating duct, pipe, pump, crack, doorway, etc.) and a number of supplementary data items defining parameters associated with that component type. When a certain flow component is repetitively present in the network, it need only be defined once. The currently supported fluid flow component types are summarized in Table 3. Detailed information can be found elsewhere (Hensen 1990).

<table>
<thead>
<tr>
<th>Code</th>
<th>Type</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Power law volume flow resistance element</td>
<td>3</td>
</tr>
<tr>
<td>15</td>
<td>Power law mass flow resistance element (definition 1.)</td>
<td>3</td>
</tr>
<tr>
<td>17</td>
<td>Power law mass flow resistance element (definition 2.)</td>
<td>3</td>
</tr>
<tr>
<td>20</td>
<td>Quadratic law volume flow resistance element</td>
<td>3</td>
</tr>
<tr>
<td>25</td>
<td>Quadratic law mass flow resistance element</td>
<td>3</td>
</tr>
<tr>
<td>30</td>
<td>Constant volume flow rate element</td>
<td>2</td>
</tr>
<tr>
<td>35</td>
<td>Constant mass flow rate element</td>
<td>2</td>
</tr>
<tr>
<td>40</td>
<td>Common orifice flow element</td>
<td>3</td>
</tr>
<tr>
<td>50</td>
<td>Laminar pipe flow element</td>
<td>3</td>
</tr>
<tr>
<td>110</td>
<td>Specific air flow opening</td>
<td>1</td>
</tr>
<tr>
<td>120</td>
<td>Specific air flow crack</td>
<td>2</td>
</tr>
<tr>
<td>130</td>
<td>Specific air flow door</td>
<td>4</td>
</tr>
<tr>
<td>210</td>
<td>General flow conduit (duct or pipe)</td>
<td>6</td>
</tr>
<tr>
<td>220</td>
<td>Conduit ending in converging 3-leg junction &amp; (C = f(q/qc))</td>
<td>13</td>
</tr>
<tr>
<td>230</td>
<td>Conduit starting in diverging 3-leg junction &amp; (C = f(q/qc))</td>
<td>13</td>
</tr>
<tr>
<td>240</td>
<td>Conduit ending in converging 4-leg junction &amp; (C = f(q/qc))</td>
<td>17</td>
</tr>
<tr>
<td>250</td>
<td>Conduit starting in diverging 4-leg junction &amp; (C = f(q/qc))</td>
<td>17</td>
</tr>
<tr>
<td>310</td>
<td>General flow inducer (fan or duct)</td>
<td>7</td>
</tr>
<tr>
<td>410</td>
<td>General flow corrector (damper or valve)</td>
<td>17</td>
</tr>
<tr>
<td>420</td>
<td>Flow corrector with polynomial local loss factor</td>
<td>16</td>
</tr>
<tr>
<td>450</td>
<td>Ideal (frictionless) flow controller</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 3 Currently available fluid flow component types

Within ESP each flow component has a subroutine counterpart which is used to generate the flow and flow derivative at each iteration. As an example, consider the type 420 component: this is a special case of a valve/damper which is described in terms of a variable dynamic local loss factor \(C\) - that is, the valve/damper is approached as if it were a conduit with local dynamic losses dependent on the correctors relative position (i.e., valve stem displacement or damper blade angle). The mass flow rate \(\dot{m}\) is calculated from:

\[ \dot{m} = \frac{2p \Delta P}{C} \left( \frac{kg}{s} \right) \]

with \(C = a_0 + a_1 H/H_{100} + a_2 (H/H_{100})^2 + a_3 (H/H_{100})^3\) (-)

where \(A\) is the cross-sectional area containing the corrector \((m^2)\), \(C\) is a factor representing local dynamic losses (-), \(H/H_{100}\) is the relative valve/damper position (-), and \(a_i\) are fit coefficients (-).
Within ESP this equation will be used to determine the related branch flow at each iteration step. As will be explained later the ESP solver also requires the partial derivative which for the case of Equation 12 is given by:

\[
\frac{\partial \dot{m}}{\partial \Delta P} = \frac{5 \dot{m}}{\Delta P} \quad (kg/s/Pa)
\]  

(14)

If \(\Delta P\) becomes too small, and in the case of flow components for which an analytical expression for the derivative does not exist, ESP will determine the value of the derivative by numerical approximation:

\[
\frac{\partial \dot{m}}{\partial \Delta P} \approx \frac{\dot{m} - \dot{m}^\%}{\Delta P - \Delta P^\%} \quad (kg/s/Pa)
\]  

(15)

where \(^\%\) denotes the previous iteration step value.

To be able to use this flow component as the actuator of a flow control mechanism, necessitates that there is also a control signal and some control law which translates sensor output into actuator input. The control law is described by the user definable parameters: day type index, start hour, finish hour, valve position outside control period, signal lower limit, relative position at low signal, signal upper limit, relative position at high signal, hysteresis, and sensed property index indicating one of: any building/plant control signal generated by ESPbops (only available in the encapsulated version of ESPfmfs), nodal temperature, signed or absolute nodal temperature difference, nodal pressure, signed or absolute nodal pressure difference, signed or absolute mass flow rate, wind speed, wind direction, diffuse or direct solar radiation, or relative humidity of outdoor air.

### 2.3 Defining Networks

The connections data defines the flow network. Each connection is described in terms of the name of the node on its (arbitrarily declared) positive side, the height of the positive linkage point relative to the node on the positive side, the name of the node on the (arbitrarily declared) negative side of the connection, the height of the negative linkage point relative to the node on the negative side, the name of the connecting flow component and supplementary data which depends on the flow component selected. Note that more than one connection may exist between two nodes so that a connection joining node A to B is different from one joining B to A. The concept of a connection having a positive side and a negative side is used to keep track of the direction of fluid flow. For most mass flow component types, uni-directional fluid flow will result (in either direction). However, some component types may represent bi-directional fluid movement - for example in the case of a doorway where, due to the action of small density variations, over the height, bi-directional flow may exist.

### 3 NETWORK SOLUTION

Each fluid flow component, \(i\), relates the mass flow rate, \(\dot{m}_i\), through the component to the pressure drop, \(\Delta P_i\), across it. Conservation of mass at each internal node is equivalent to the mathematical statement that the sum of the mass flows must equal zero at such a node. Because these flows are non-linearly related to the connection pressure difference, solution requires the iterative processing of a set of simultaneous non-linear equations subjected to a given set of boundary conditions. The technique employed by ESP is to assign an arbitrary pressure to each internal node to enable the calculation of each connection flow from the appropriate connection equation. The internal node mass flow residuals are then computed from:
where \( R_i \) is the node \( i \) mass flow residual for the current iteration \((\text{kg/s})\), \( \dot{m}_k \) is the mass flow rate along the \( k \)th connection to the node \( i \) \((\text{kg/s})\) and \( K_{i,i} \) is the total number of connections linked to node \( i \).

The nodal pressures are then iteratively corrected and the mass balance at each internal node is re-evaluated until some convergence criterion is met. The method used in ESP is based on an approach suggested by Walton (1988). This approach was implemented and tested in an earlier version of ESP and shown to result in considerable speed improvements as evidenced in table 4 (Clarke & Hensen 1988).

### Table 4: Bench-mark results

<table>
<thead>
<tr>
<th>Problem</th>
<th>Original Solver</th>
<th>New Solver</th>
<th>24 hr CPU Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CPU Seconds</td>
<td>Iterations 1st hr - 24 hrs</td>
<td>CPU Seconds</td>
</tr>
<tr>
<td>1. atria</td>
<td>3087</td>
<td>6363 - 152117</td>
<td>55</td>
</tr>
<tr>
<td>2. house 1</td>
<td>377</td>
<td>374 - 27863</td>
<td>17</td>
</tr>
<tr>
<td>3. house 2</td>
<td>48</td>
<td>146 - 2510</td>
<td>23.2</td>
</tr>
<tr>
<td>4. 2 zone</td>
<td>9</td>
<td>309 - 2376</td>
<td>3.6</td>
</tr>
<tr>
<td>5. 3 zone</td>
<td>3</td>
<td>27 - 358</td>
<td>2.5</td>
</tr>
<tr>
<td>6. Trombe</td>
<td>2138</td>
<td>14009 - 122754</td>
<td>50.2</td>
</tr>
<tr>
<td>7. large</td>
<td>13270</td>
<td>25318</td>
<td>24 - 1</td>
</tr>
</tbody>
</table>

The latest ESP model has a further enhanced solver which has resulted in additional iteration reductions. However, at the time of writing no bench-mark results were available. The solution method is based on a Newton-Raphson technique applied to the set of simultaneous nonlinear equations (for example see Conte and De Boor 1972). With this technique a new estimate of the vector of all node pressures, \( \mathbf{P}^* \), is computed from the current pressure field, \( \mathbf{P} \), via:

\[
\mathbf{P}' = \mathbf{P} - \mathbf{C}
\]

where the node pressure correction vector, \( \mathbf{C} \), is determined on the basis of a simultaneous solution of a Jacobian matrix which represents the nodal pressure corrections in terms of all branch flow partial derivatives. The pressure corrections vector \( \mathbf{C} \) is given by:

\[
\mathbf{C} = \mathbf{R} \mathbf{J}^{-1}
\]

where \( \mathbf{R} \) is the vector of nodal mass flow residuals and \( \mathbf{J}^{-1} \) is the inverse of the square Jacobian matrix \((N^2 \times N^2)\) for a network of \( N \) nodes) whose diagonal elements are given by:

\[
J_{n,n} = \frac{\sum_{k=1}^{K_{n,n}} \frac{\partial \dot{m}_n}{\partial \Delta P_k}}{(\text{kg/s Pa})}
\]

(19)

where \( K_{n,n} \) is the total number of connections linked to node \( n \) and \( \Delta P_k \) is the pressure difference across the \( k \)th link. The off-diagonal elements of \( \mathbf{J} \) are given by:

\[
J_{n,m} = \frac{\sum_{k=1}^{K_{n,m}} \frac{\partial \dot{m}_m}{\partial \Delta P_k}}{(\text{kg/s Pa})}
\]

(20)

where \( K_{n,m} \) is the number of connections between node \( n \) and node \( m \). This means that - for internal nodes - the summation of the terms comprising each row of the Jacobian matrix are identically zero.
ESP currently uses LU decomposition with implicit pivoting (also known as Crout's method with partial pivoting) for solution of the matrix equation \( J \mathbf{C} = \mathbf{R} \) for the unknown pressure correction vector \( \mathbf{C} \). The implementation in use by ESP originates from an algorithm by Press (et al. 1986). In this case the matrix \( J \) is decomposed to a lower triangular matrix \( \mathbf{L} \) and an upper triangular matrix \( \mathbf{U} \), such that \( \mathbf{L} \mathbf{U} = \mathbf{J} \). This decomposition is used to solve the linear set:

\[
J \mathbf{C} = (\mathbf{L} \mathbf{U}) \mathbf{C} = \mathbf{L} (\mathbf{U} \mathbf{C}) = \mathbf{R}
\]

by first solving, by forward substitution, for the vector \( \mathbf{Y} \) such that \( \mathbf{L} \mathbf{Y} = \mathbf{R} \) and then solving (by back substitution) \( \mathbf{U} \mathbf{C} = \mathbf{Y} \). The advantage is that both substitutions are quite trivial. Pivoting is used to make the method numerically stable.

As a future possibility, sparse matrix methods could be used to reduce further the storage and execution time requirements.

It should be noted that it is quite easy to define a mass flow network which has no unique solution. One requirement for solution is that at least one of the node pressures is known. A second requirement is that all nodes must be linked, through some path, to a known pressure node.

Conservation of mass at each internal node provides the convergence criterion. That is, if \( \sum Q_i = 0 \) for all internal nodes for the current system pressure estimate, the exact solution has been found. In practice, iteration stops when all internal node mass flow residuals are below one of two user definable thresholds: \( \text{ERRMAX} \) the largest percentage residual flow error, or \( \text{FLOMAX} \) the largest absolute residual flow error.

In some cases, large corrections for the successive pressure correction applied to any node during the iteration process may cause a numerical instable situation. Therefore, ESP offers \( \text{PMAX} \) a user definable maximum pressure correction applied to any node during the iteration process.

![Figure 3 Example of successive computed values of pressure and oscillating pressure correction at a single node](image)

As noted by Walton (1988), there may be occasional instances of low convergence with oscillating pressure corrections on successive iterations at a single node. In the case shown in Figure 3, each successive pressure correction is a constant ratio of the previous correction - that is \( C_i = -0.5 \times C_i^{\text{prev}} \) (\( \text{prev} \) denotes the previous iteration step). In a number of tests the observed oscillating corrections came close to such a pattern. By assuming a constant ratio, it is simple to extrapolate to the ‘final solution’:

\[
P_i^* = P_i - C_i / (1 - r) \quad (Pa)
\]

where \( r \) is the ratio of \( C_i \) for the current iteration to its value in the previous iteration. The factor \( 1 / (1 - r) \) is called a relaxation factor. The extrapolated value of node pressure can be used in the next iteration. If it is used, then \( r \) is not evaluated for that node in the following iteration but only in the one thereafter. In this way, \( r \) is only evaluated with unrelaxed pressure.
correction values. This process is similar to Steffensen iteration (Conte and De Boor 1972) which may be used with a fixed point iteration method for individual non-linear equations. The iteration correction method presented above gives a variable and node dependent relaxation factor. When the solution is close to convergence, Newton-Raphson iteration converges quadratically. By limiting the application of the relaxation factor to cases where $r$ is less than some value (ESP's user definable parameter STEFFR) such as -0.5, it will not interfere with the rapid convergence.

4 COMBINED HEAT AND MASS FLOW SIMULATION

Within the ESP system, a fluid flow simulation may be initiated independently of the main energy simulation or pursued in tandem. In the former case the assumption is made that the flows are predominantly pressure driven and that buoyancy effects, although included, are time invariant (or user specifiable). In the latter case ESP must establish and solve the coupled, matrix equations corresponding to the heat and fluid flows within the multi-zone building and the multi-component plant. The ESP scheme, which is reported fully elsewhere (Clarke 1990), can be summarised, for any computational time-step, as follows.

- the energy balance, state-space equations corresponding to the finite volumes which represent the plant-side discretised components and distribution network are established on the basis of the latest values of the building-side state variables and plant component/network mass flows
- this plant matrix equation is then solved by a sparse matrix technique taking into account any defined control action
- the energy balance, state-space equations corresponding to the finite volumes which represent the building-side discretised constructions, surfaces and air volumes are then established on the basis of the latest values of the plant flux inputs and building-side air flows
- this building matrix equation is then solved by a customised matrix inversion technique which employs a partitioning and ordering technique which ensures that only non-zero matrix entries are processed and which integrates control system characteristics within the solution process
- the whole-system, fluid flow equations are then solved, iteratively, by the technique described earlier in this paper, utilising the newly established building and plant-side state variables to estimate the buoyancy effects
- if required, time-step control can be activated to prevent the evolution of time in cases where the newly computed state-variables differ markedly from the latest values assumed when the matrix equations were established
- finally, the simulation clock is incremented and the process repeats

Since the time constant associated with the state-space equations representing plant-side finite volumes are often an order of magnitude smaller than their building-side counterpart, a facility is provided to allow the plant system equations to be established and solved at a greater frequency than the building system equations.

5 A CASE STUDY

In a paper by Emslie (1990) four case studies are presented involving air infiltration modelling in buildings with ESP. These case studies were selected from a portfolio of computer modelling projects carried out by the Energy Design Advisory Service (Emslie & Chalmers 1988).

One of the case studies was concerned with thermal upgrading of Ladywell high rise, a tower block in Glasgow comprising a number of similar 1 and 2 bedroom flats. A detailed computer
Figure 4 Plan view and air leakage network of 1 bedroom flat

Simulation study was commissioned to predict the most cost-effective options for upgrading in terms of occupant comfort, condensation risk, heating capacity required and energy consumption & cost. As part of the study it was necessary to predict 'design' air infiltration rates for all rooms in two cases: (i) leaving existing ill fitting single glazing units unmodified or, (ii) replacing with new double glazed units incorporating trickle ventilators. Given the site microclimate details, it was decided that infiltration rates be predicted for two wind directions.

<table>
<thead>
<tr>
<th>flat</th>
<th>glazing</th>
<th>wind</th>
<th>living</th>
<th>kitchen</th>
<th>hall</th>
<th>bath</th>
<th>bed 1</th>
<th>bed 2</th>
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<td></td>
<td>1.6</td>
<td>1.1</td>
<td>0.0</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 5 Ladywell high rise: predicted 'design day' average air infiltration rates (air changes per hour) for 1 and 2 bedroom flats

Figure 4 shows a plan view of the 1 bedroom flat with the distributed air leakage network (consisting of windows, cracks, doors) superimposed. Design day simulation using representative hourly weather data for Glasgow gave hourly nodal pressure distribution and leakage path's air flow rates. ESP offers facilities to retrieve this data both tabular and graphical. It is also possible to reduce this data to predicted average air infiltration rates for each flat type as listed in Table 5.

These simulations demonstrated the effect on air infiltration to be expected from window replacement. With regard to the global study, which involved detailed thermal modelling as well as air flow modelling, it was concluded that in this case window replacement outperformed proposed wall insulation upgrading as a means of energy conservation.

6 CONCLUSIONS

This paper has demonstrated how a mass flow network method can be used to provide a unified model of major building and plant fluid flows. It was shown how this model can be used for the simulation of coupled heat and mass flows in buildings. The performance of the model indicates that it is practical to solve the building/plant heat and mass flow network in detail. Solution of complex fluid flow networks for problems involving many time steps is now feasible on current small computers.

It is felt that the model reflects the current state of the art in the field of network modelling approach to simulation of coupled heat and mass flows in buildings. Development of the model did reveal however that research is still needed in several areas. These include development of additional fluid flow component models (especially improved large opening models), modelling
of intrazone effects by simplified methods and by integration with CFD modelling methods, expansion of the wind pressure database, expansion of the actual building and plant components 'database', and experimental validation of the simplifying assumptions in the flow component models and the network method.

Acknowledgements
The authors are indebted to George Walton who so willingly shared his theoretical approach to the simulation of air flow in buildings.

References
Discussion
Paper 45

J.Axley (MIT, USA)

The source reference for Figure 2 in the paper is erroneous.

J.Hensen (Technische Universiteit, Eindhoven, Netherlands)

In our paper we reference the AIRNET report by G. Walton as the source for the figure and for the way in which stack effects are handled. Since the report in question did not state otherwise, we naturally assumed this to be the original source. From Walton’s final paper on AIRNET at the 1989 ASHRAE summer meeting, it is now clear that a number of the ideas used in that model also originate from Dr. J. Axley.

J.Axley (MIT, USA)

There is a need to provide linear flow equations for low flow ranges of components to avoid near singularity of the system Jacobian thereby avoiding convergence problems for low flow cases.

J.Hensen (Technische Universiteit, Eindhoven, Netherlands)

in ESPmfs, low flow cases do not impose problems. Even zero flow cases are handled correctly. Therefore we do not think that it is necessary to provide separate expressions for low flow cases. Furthermore, linear equations can only be provided for a number of component types (it is for instance impossible in case of a black box (perhaps look-up table) component.

J.Axley (MIT, USA)

It can be proven that the system of non-linear flow equations results in a positive definite nonsingular matrix. The solution method will be numerically stable, regardless of the fact whether pivoting is used or not.

J.Hensen (Technische Universiteit, Eindhoven, Netherlands)

We agree on the first part of the statement. Regarding the necessity of (partial) pivoting we do not agree, and refer to the following quote from Press et al (1986) from their Section 2.3 on the LU decomposition method: “Pivoting is absolutely essential for the stability of Crout’s method. Only partial pivoting (interchange of rows) can be implemented efficiently. However this is enough to make the method stable”...

J.Axley (MIT, USA)

Linear expressions used for the low-flow range provide a convenient means to initialize solution strategy.

J.Hensen (Technische Universiteit, Eindhoven, Netherlands)

See question two above. Furthermore, we found that in ESPmfs’s case of successive time steps the pressures for the previous time step usually give a pretty good initial pressure vector for the next step.

J.Axley (MIT, USA)

Did you have a look at the paper/poster by R.A. Grot and J.Axley on “Structure of models for the prediction of air flow and contaminant dispersal in buildings”?

J.Hensen (Technische Universiteit, Eindhoven, Netherlands)

Because the paper by Axley and Grot was not included in the Conference preprints and at the time of presentation it was very crowded at the poster session, I did not have any real opportunity to study the paper/poster in great detail. Furthermore, I lost the point which Dr.Axley was trying to make with his comment. From another recent paper by Axley and Grot (1989) I think it might have been the fact that we do not use an integral element formulation approach to coupled airflow analysis and thermal analysis which is described in that paper. Although I think that what is described is a very interesting approach - especially in view of current software engineering developments like the object orientated approach - we did not consider a similar approach at this point in time. The main reasons being: although the emphasis in our paper was on simulation of air flow, ESPmfs is really developed for a wider field of interest including different fluids and a broad spectrum of plant components. I am not sure whether it will be easy or even possible to establish in all cases the kind of element equations which Axley and Grot describe (e.g. in case of a component which is only described in terms of certain input/output relationships) - ESP uses 5 basic
matrix equations: for building side energy, plant side energy, plant side 1st phase mass flow rate, plant side 2nd phase mass flow rate and for the combined building and plant mass flow network, respectively. Combining these matrix equations into 1 is particularly useful if it is possible to use a direct solution method. In case of non-linear relationships between state-variables or non-linear control strategies - like we have - a direct method is not possible. If you use an indirect (say iterative) method, it does not seem to make much difference whether you use one combined or several separate matrix equations. On the other hand, if you do use the separate matrix approach it is very easy to introduce mixed-frequency and variable time stepping schemes. In that case it is also quite easy to exclude certain matrix equations if they are of no interest in a certain problem context (e.g. the mass flow network matrix in case the flows are constant) - introducing the method described by Axley and Grot would involve complete restructuring of the main simulation engine, while incorporating the method as described in our paper was relatively straightforward.

B A Fleury, ENTPE-LASH, France

I wonder about the difference between ESPair, the air flow network model already present in the ESP system, and the model described in the current paper, ESPmfs. Also, the coupling between energy and air flow.

J Hensen (Technische Universiteit Eindhoven, Holland)

Some of the differences between ESPair and ESPmfs are already indicated above. ESPmfs is a completely new development, which is set up in a highly modular fashion to facilitate easy introduction of new flow component models, alternative matrix solvers, etc. When compared to ESPair, the main differences, in terms of functionality are: ESPmfs is a general building and plant fluid mass flow network solver, whereas ESPair is restricted to air flow through a very limited number of building opening type air leakage models. ESPmfs offers more node types and eg. alternative theories with respect to wind pressure calculation. The stack effect calculation is quite different. The coupled heat and mass flow simulation is now extended to the plant side. In terms of solution method the main difference is that ESPair uses a node wise Newton-Raphson method, while ESPmfs uses a whole network NR approach. In terms of performance the main differences are illustrated by the speed improvements as indicated in Table 4. The coupling between energy flow and air flow is basically established by substituting the appropriate fluid mass flows in the whole building energy matrix coefficients with the mass flows calculated by the in ESPbps incorporated version of ESPmfs at each finite calculation time step.