AIR MOVEMENT & VENTILATION CONTROL WITHIN BUILDINGS

12th AIVC Conference, Ottawa, Canada
24-27 September, 1991

POSTER 37

SIMULTANEOUS CALCULATION OF AIRFLOWS, TEMPERATURES AND CONTAMINANT CONCENTRATIONS IN MULTI-ZONE BUILDINGS

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SYNOPSIS

The computer programs published so far have enabled the calculation of airflows at constant temperatures or of air temperatures at constant airflows.

The first version of a new microcomputer program has now been developed in which the airflows and temperatures are calculated simultaneously. The time-dependency of temperatures, airflows and contaminant concentrations is considered in the calculation method. The source strength of contaminants, outdoor air temperature, wind velocity and direction, convection and radiation loads can all be freely scheduled. The supply air temperature in mechanical ventilation can be selected as: (1) constant (and scheduled), (2) equal to that of the outdoor air, (3) calculated as the temperature of the mixture of outdoor air and return air.

Constant-temperature cases were simulated with the program and the results compared with those obtained from more sophisticated programs. Other cases, with variable temperatures, were compared with the measurements. Good agreement of the results was obtained in all cases.

The paper describes the main features of the new program and gives some simulation results.

NOMENCLATURE

A	=	area of opening, (m^2),
A	=	flow coefficient, (m^3/s at 1 Pa),
A_w	=	surface area of wall, (m^2),
A_{ij}	=	section area of flow path from node i to node j, (m^2),
A_{ww}	=	surface area of window, (m^2),
a	=	dummy variable,
B	=	flow exponent,
C_1	=	constant,
C_2	=	constant,
C_d	=	discharge coefficient, (-),
C_i	=	concentration of contaminant in space associated with node i, (kg/m^3) or (pol) or (vol. ppm),
C_i	=	thermal capacity of air in zone i, (J/K),
C_{iw}	=	thermal capacity of wall w in zone i, (J/K),
c_p	=	specific thermal capacity of air, (J/kgK),
D	=	equivalent diameter of duct, (m),
F'	=	function,
F''	=	nonlinear function,
f_1	=	friction loss factor, (-),

f_2 = local pressure loss factor, (-),

G_i = constant strength of contaminant source placed at node i, (kg/s) or (olf) or (L/h),

H = height of opening, (m),

K_{ij} = general coefficient of pressure loss,(-),

L_{ij} = length of flow path from node i to node j, (m),

L = length of duct, (m),

m_{ij} = mass flow of air from node i to node j, (kg/s),

p_i = absolute pressure at node i, (Pa),

p_u = pressure difference that accounts for the effect of turbulence, (Pa),

p_x = pressure difference that generates the net flow through large opening, (Pa),

Δp = pressure difference, (Pa),

Q_c = thermal load by convection, (W),

Q_r = thermal load by radiation, (W),

q = volume airflow, (m^3/s),

q_1 = air inflow, (m^3/s),

q_2 = air outflow, (m^3/s),

q_{ij} = volume flow of air from node i to node j, (m^3/s),

S_{ij} = stack effect in flow path from node i to node j; head generated by fan, (Pa),

T_i = temperature of air in zone i, (°C),

T_{iw} = surface temperature of wall w in zone i, (°C),

T_o = outdoor air temperature, (°C),

T_{iwx} = temperature of air in zone on opposite side of wall w in zone i, (e.g. outdoor air temperature for external wall), (°C),

T_w = temperature of surface of wall, (°C),

T_{wr} = temperature of surface of hemisphere, (°C),

ΔT = temperature difference, (K),

t = time, (s),

U_{iw} = overall heat transfer coefficient of wall w in zone i, (W/m^2K),

U_{ww} = overall heat transfer coefficient of window, (W/m^2K),

V_i = volume of space associated with node i, (m^3),

v = velocity of airflow, (m/s),

v_x = mean air velocity corresponding to net flow rate through large opening, (m/s),

W = width of the opening, (m),

α_c = film heat transfer coefficient by convection, (W/m^2K),

α_r = film heat transfer coefficient by radiation, (W/m^2K),

ρ = air density, (kg/m^3),

ρ_m = mean air density, (kg/m^3),

1. INTRODUCTION

A number of programs have been developed recently for predicting contaminant concentrations, e.g. [2, 13], for the thermal simulation of buildings, mainly with respect to energy analysis, e.g. [1], and for calculating the airflows in a building, e.g. [16]. The state of the art is to the best of the authors' knowledge represented by: CONTAM [2] for concentration prediction, AIRNET [16] combining infiltration, airflows and ventilation ducting, and DTFAM [3] considering coupled airflow and thermal analysis (not yet released).

The thermal capacity of the building structure has an effect on the indoor air temperature. There is a link between the air temperature and air flows. Airflows are the major distribution routes by which contaminants spread throughout the building. Therefore, the airflows and air temperatures should be taken into consideration in predicting contaminant concentrations in the building.

None of the available programs is alone capable of simultaneously calculating contaminant concentrations, airflows and air temperatures. This fact provided the main stimulus for the research work presented here. The aim of the study was to develop the first version of a computer program for predicting contaminant concentrations in buildings making simultaneous allowance for airflows and the thermal behaviour of the building structure in dynamically changing conditions. The program was intended for microcomputer to enable simulations covering a period of one or two days.

The following is a brief report of the fundamentals of the models used in the program and some simulation results.

2. GENERAL

The program is called TFCD. The letters in the abbreviation contain information on what the program does - it calculates Temperatures, air Flows, Concentrations of contaminant and air quality in terms of Predicted Percentage of Dissatisfied (PPD) due to contaminant concentration.

The source code of the program, listed in [8], is written in Fortran 77. Figure 1 depicts the sequence in which the computations are performed by the program.

The simulated building is modelled by a network whose branches represent airflow routes and its nodes refer to the volumes (zones). The program is at present capable of simulating a system consisting of at most 40 nodes.

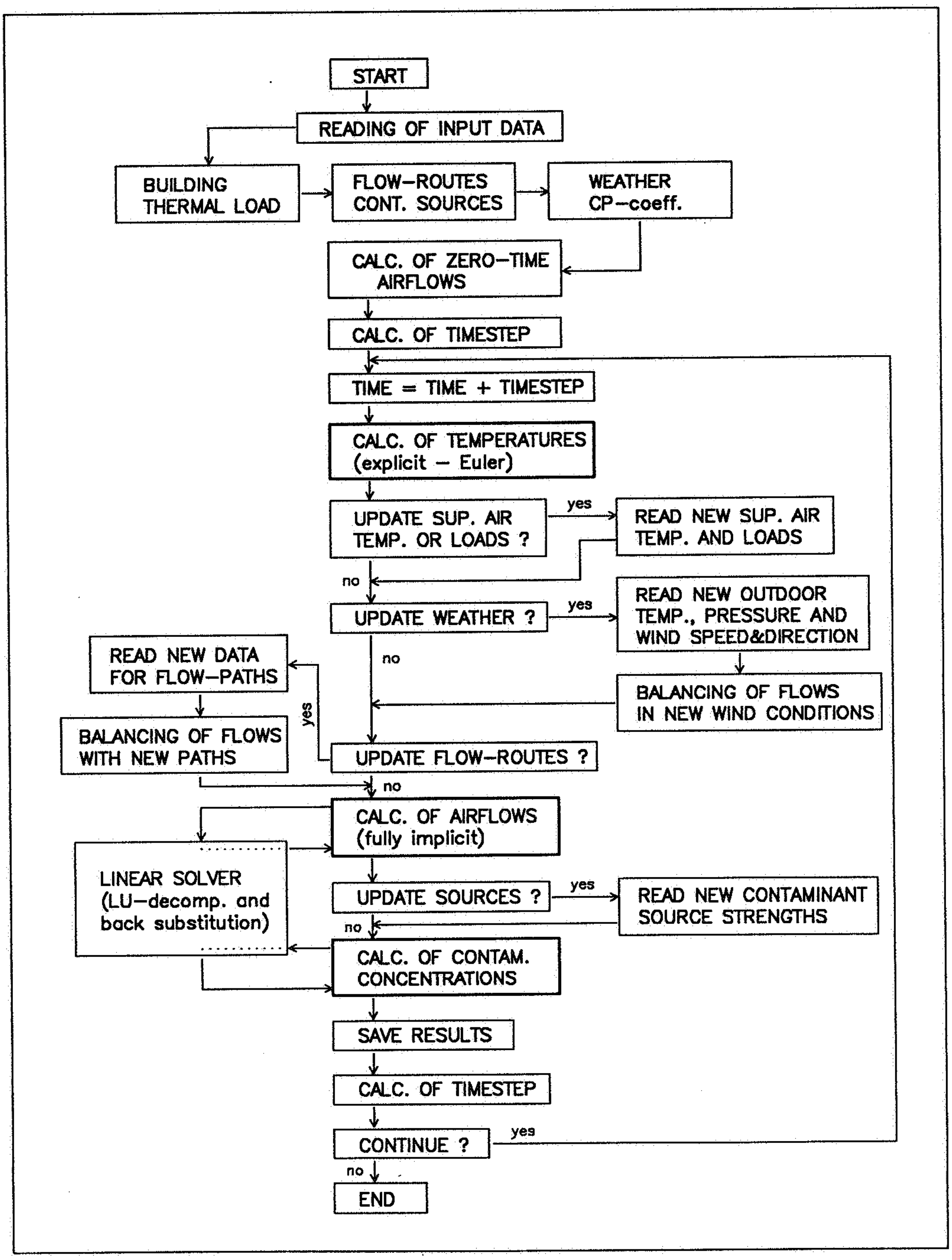


Figure 1. A simplified block diagram of the program.

In order to enable the simulation of cases resembling reality as well as possible, the following options are provided for use in the program :

- outdoor air temperature - constant, changing according to sine function in 24 hour period, changing stepwise with a free schedule;
- barometric pressure, wind speed and direction - constant, changing with a free schedule;
- supply air temperature of mechanical ventilation - constant, changing stepwise with a free schedule, equal to outdoor air temperature, equal to the temperature of a mixture of outdoor air and return air (if such is used);
- thermal loads by convection and radiation - constant, changing stepwise with a free schedule;
- strengths of contaminant sources - constant, changing stepwise with a free schedule;
- type and pressure-flow characteristics of airflow routes - constant, changing with a free schedule (change of type limited, see Appendix 2 in [8]).

3. CALCULATION OF TEMPERATURES

An extended version of the thermal model presented in [5] was applied for calculation of the air temperatures at the indoor nodes of building network. Each room in the building was considered as one or more zones vertically stacked. One network node was placed in each zone. It was assumed that the air inside the zone is instantly and perfectly mixed. The set of differential equations was written for each zone :

$$\frac{dT_i}{dt} C_i = \sum_j m_{ji} c_p (T_j - T_i) + \sum_{iw} \alpha_c A_{iw} (T_{iw} - T_i) + \sum_{ww} U_{ww} A_{ww} (T_o - T_i) + Q_c \qquad (1)$$

$$\frac{dT_{iw}}{dt} C_{iw} = A_{iw} (T_{iwx} - T_{iw}) \left[\frac{1}{U_{iw}} - \frac{1}{\alpha_c + \alpha_r} \right]^{-1} + Q_r + \alpha_c A_{iw} (T_i - T_{iw}) + \alpha_r A_{iw} (T_{iwr} - T_{iw}) \qquad (2)$$

The set for a node has one equation (1) and as many equations (2) as there are walls (10=max.) associated with the node in question.

Whereas the thermal capacity of the zone air is calculated at each time step, the thermal capacity of the wall is approximated by one constant. Since it is related to the duration of the simulation, the wall capacity will obtain different values depending on the application.

The Euler method was chosen for solving the temperatures. Advantages of this are the minimal computational effort required to find temperatures and the fact that there is no need for iterations between temperatures and airflows. The stability analysis is then inevitable. However, the cost is ultimately an advantage because the upper limit for the time step emerges automatically from stability analysis. Thus the user of the program is not faced with the cumbersome task of deciding the length of the time step to be used in simulation.

4. CALCULATION OF AIRFLOWS

4.1. Numerical model of building network

The building is considered as a set of nodes connected by the branches of the network. Network nodes are placed at the external envelope, at both ends of the flow paths in the ducting, and in the indoor zones of the building.
The wind pressure acting on the external nodes, fans in the air handling system and buoyancy create pressure differences between the nodes of the network.

For each network node in the ventilation ducting and indoor zones of the building, the following differential equations are written [7]

$$V_i \frac{d\rho_i}{dt} + \sum_j m_{ij} = 0 \qquad (3)$$

$$\frac{L_{ij}}{A_{ij}} \frac{dm_{ij}}{dt} - p_i + p_j + \frac{1}{2} K_{ij} |m_{ij}| m_{ij} = S_{ij} \qquad (4)$$

Equations (3) and (4) must both be fulfilled for all the nodes simultaneously. This model was first adapted for calculating the airflows in the building in computer code SMOV [15].

The model based on eqs. (3) and (4) predicts the airflows as one-way flows. A separate model is used in the program for calculating two-way flows through large openings.

In order to obtain the solution, the differential eqs. (3) and (4) must be discretized. Fully implicit discretization avoids potential stability problems. Equations (3) and (4) are discretized and linearized as shown in [7]. The linear matrix equation is created and solved in the program by means of standard LU-decomposition and the back substitution method [10].

The general coefficient of pressure loss, K_{ij} in model eq. (4), is calculated from the equation

$$0.5\ K_{ij}\ m_{ij}^{2} = \Delta p_{ij} \qquad (5)$$

The coefficient K_{ij} is calculated in a different way depending on the pressure-flow characteristics of the flow path. At present the program is able to handle nine types of flow paths. Their characteristics are provided in the appendix.

4.2. Calculation of two-way flows

The model [13] used in the program to calculate the two-way airflows through large openings consists of a large number of equations that may be written in general form as :

$$q_1 = C_1\ C_d\ W\ H \cdot F'\{a,H\} \cdot F_1''\{p_x, p_u, \rho_m, a, H\} \qquad (6)$$

$$q_2 = C_2\ C_d\ W\ H \cdot F'\{a,H\} \cdot F_2''\{p_x, p_u, \rho_m, a, H\} \qquad (7)$$

The difference between the outlow q_2 and the inflow q_1 is the net flow

$$q_2 - q_1 = q_{net} \qquad (8)$$

The discharge coefficient, C_d, is calculated from the formula

$$C_d = 3.7v_x + 6.4v_x e^{-\Delta T} - 0.9e^{-\Delta T} + 0.96 \qquad (9)$$

where :

$$v_x = q_{net} / (H\,W) \quad . \tag{10}$$

Equation (9) was derived from the results of tracer gas measurements and is valid for [13]

$0 \le v_x \le 0.05$ m/s and $0 \le \Delta T \le 3.0$ K .

The values for constants C_1, C_2 and the forms of functions F' and F'' in eqs. (6) and (7) are obtained in the program by selecting applicable equations from the model set, see [13] for precise formulation of the equations. Appropriate equations are identified depending on the position of neutral levels, the temperature difference between the spaces and the values of the pressure differences.

5. CALCULATION OF CONTAMINANT CONCENTRATIONS

5.1. Numerical model and solution method

The numerical model for calculating contaminant concentrations is based on a simple differential equation of contaminant mass balance similar to eq. (3) for air. It was assumed that the contaminant is instantly and perfectly mixed with the air and is passive.

Once the airflows have been determined, the balance equation of the mass for contaminant may be written for each node of the building network. It is discretized as [12] :

$$\frac{C_i^{(t)} - C_i^{(t-\Delta t)}}{\Delta t} V_i = G_i + \sum_{j=i} q_{ji} C_j^{(t)} - \sum_{j=i} q_{ij} C_i^{(t)} \tag{11}$$

The superscript $(t-\Delta t)$ refers to the value at the previous time step and (t) refers to the value at the present time step.

Equation (11) is rearranged to obtain a linear matrix equation that is solved for the vector of concentrations by means of the same solver (standard LU-decomposition and back substitution method) as was previously used to determine the airflows.

5.2. Evaluation of air quality

Three units may be used in the program for calculating the contaminant concentrations (kg/m^3, ppm, pol).

The perceived air quality may be quantified in terms of Predicted Percentage Dissatisfied [6] as :

$$PPD = 395 \exp(-3.25\ C^{-0.25}) \quad \text{for } C \leq 31.3 \text{ decipol}$$

$$PPD = 100\ \% \quad \text{for } C > 31.3 \text{ decipol}$$

(12)

where C is the perceived air pollution expressed in decipols.

The air quality at each node of the network is evaluated in the program by means of eq. (12) whenever the source strengths are expressed in olfs and the concentrations in pols.

6. RELIABILITY CONSTRAINTS OF THE MODELS

The reliability of the numerical methods applied in the program was proved by means of validation cases [8]. However, comprehensive verification by means of measurements must still be conducted in order to gain general confidence in the simulation results.

At this stage, it should be pointed out that the models used in the program contain several simplifications. Some of them were necessary in order to reduce the computer memory requirements and thus to meet the aim that the program should run on a microcomputer.

The most important simplification of the thermal model is the requirement of the thermal capacity of each wall to be provided in input data, i.e. it is not calculated within the program. Advanced methods exist, involving response factors, for determining the dynamical behaviour of multi-layer walls. These methods are applicable to long-term simulations, e.g. aiming at evaluation of energy consumption in buildings, and require large memory space and computational effort. In short-term simulations only the dynamics of the active part of the wall has an impact on the space air temperature [5]. If this active part consists of one layer, its capacity may be approximated [8]. In future versions of the program some improvement allowing for the simulation of multi-layer walls should be considered.

The reliability of the model for calculating airflows is affected by the quality of the input data. For example, in spite of the fact that considerable effort has already been made to collect the wind pressure coefficients [9, 4], generally applicable data are still not available. The values of the parameters for the leakage characteristics of elements in a modelled building required by the program as input data are uncertain as long as they are not measured in situ.

Airflows between vertically stacked spaces were modelled as one-way flows. This is a rough simplification and should be updated as soon as a more advanced model is available.

The assumption of the instantaneous and perfect mixing of air and contaminant within the zone is the fundamental simplification applied in the model for calculating the contaminant concentrations in the building. It was inevitable since it is not yet known how to deal with nonuniform distribution of concentration. Due to this simplification, the choice of zones has a decisive effect on the calculated results. Usually it is correct to simulate one zone in one room. However, in some cases, particularily when the doorway is large in proportion to the size of the room, it may be useful to combine several rooms into one zone, see e.g. [14]. The only way to confirm the correctness of the choice of zones is by measurement.

The simplifications used in the models should be kept in mind since they affect the results of the simulations performed with the program.

7. EXAMPLE OF A PROGRAM APPLICATION

Part of a fictive office building was used in the simulations. The system consists of four rooms (each 4x4x3m) and a corridor, fig. 2. The corridor was divided into two equal zones (8x2x3m) with a large opening (height 3m, width 2m) between them. All the doors are 2m high and 1m wide. Convective thermal loads ranging from 7.5 W/m^2 to 30 W/m^2 are imposed on each of the rooms 13 through 16. A contaminant source of 25 olfs is placed only in room 13. The mechanical ventilation, fig. 2, aimed to represent a typical design solution.

Ventilation air is supplied to and exhausted from the rooms so that the air exchange rates in the rooms are approx. 1.85 $(m^3/h)/m^3$. The rooms are maintained at approx. 20 Pa underpressure with respect to outdoors. The corridor spaces are served only by an extract fan that maintains the corridor at approx. 0.5 Pa underpressure with respect to the rooms.

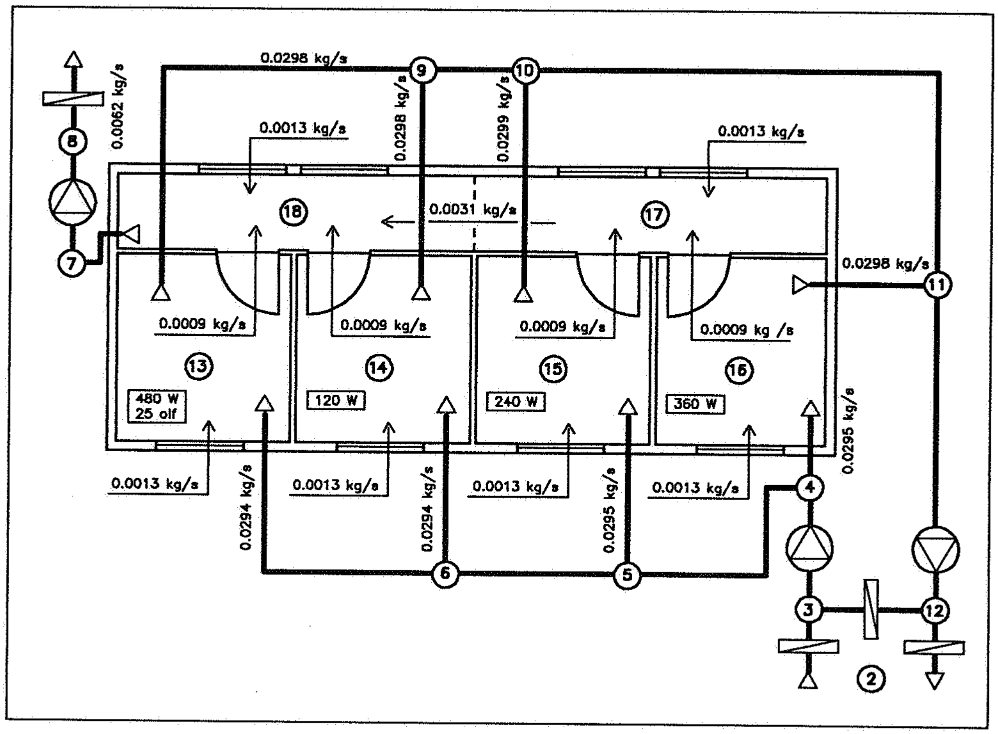


Figure 2. Layout of the simulated building.

The air enters the corridor as infiltration from outdoors and as leakages from the rooms. The doors are assumed to be of poor tightness and the windows are assumed to be relatively tight. Due to the small pressure drop across the closed door, opening the door has little effect on the balance of flows in the system.

A number of simulations were performed to determine the spread of contaminant from room 13, where it is generated, to other spaces of the system in different setups of door positions and with or without the return air. Regardless of whether the return air was used or not, the air flow rates were as shown in fig. 2. The duration of the simulations, 8 hours, depicts the length of the working day in an office building. The building was assumed to be of medium-weight construction, the temperature of the air supplied to all rooms was 17°C, the outdoor air temperature was a constant 20°C and the wind velocity was 0 m/s in all the simulations. In these conditions the airflows, air temperatures and contaminant concentrations were calculated in each zone of the simulated building. The results of the simulations are presented in figs. 3 and 4. The concentrations are expressed in terms of PPD (eq. (12)) in order to evaluate simultaneously the air quality.

7.1. First simulation

The arrangement in which all the doors were closed was used in the first simulation. The courses of the temperatures, fig. 3a, are in accordance with the thermal loads in the rooms.

A steady state of contaminant concentration in room 13 is achieved after approx. 2 hours when no return air is used, see fig. 3b. The air quality in room 13 is very poor due to the very high strength of the contaminant source. Contaminant penetrates the corridor spaces, where the steady state is not achieved and the air quality remains within the range of acceptability. Due to the design of the airflows, the other rooms remain free from contaminant.

The plot in fig. 3c shows histories of the air qualities in a simulation using 57.2% return air. Steady state concentrations in the rooms are achieved after approx. 4 hours.
It is interesting to note that the use of as much as 57.2% return air does not greatly change the concentration in room 13 compared with full-fresh air ventilation, figs. 3b and 3c. Contaminant re-entering the system with return air spreads not only to room 13 but also to other rooms, i.e. the capacity of the entire system has an impact on the concentration in room 13. Due to the use of return air, the contaminant concentrations are shifted in all spaces of the system and the resulting air qualities are not acceptable. The concentrations in rooms grow faster than those in corridors, due to the high supply air flow rates in the rooms.

7.2. Second simulation

A study was made of the effect of changing the position of the doors on the spread of contaminant throughout the system. The door of room 13, where contaminant was generated, remained open during the simulation. Other doors were simulated to be opened and closed according to the schedule shown at the bottom of fig. 4.

As long as the door of the room remains closed, the temperature grows at a rate proportional to the thermal load and the contaminant does not enter the room when return air is not used, see figs. 4a and 4c. The moment the door is opened, a relatively high temperature difference exists across the opening and powerful two-way airflows through the opening are established, see fig. 4b, where major flows are plotted.

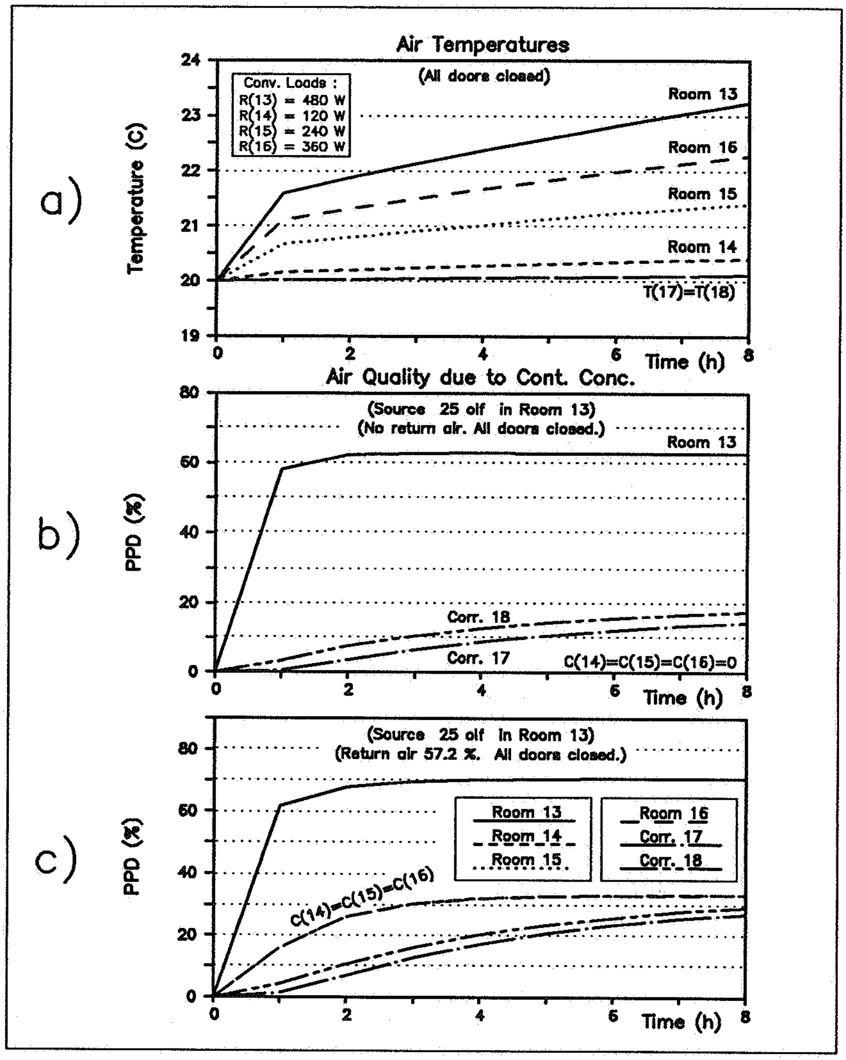
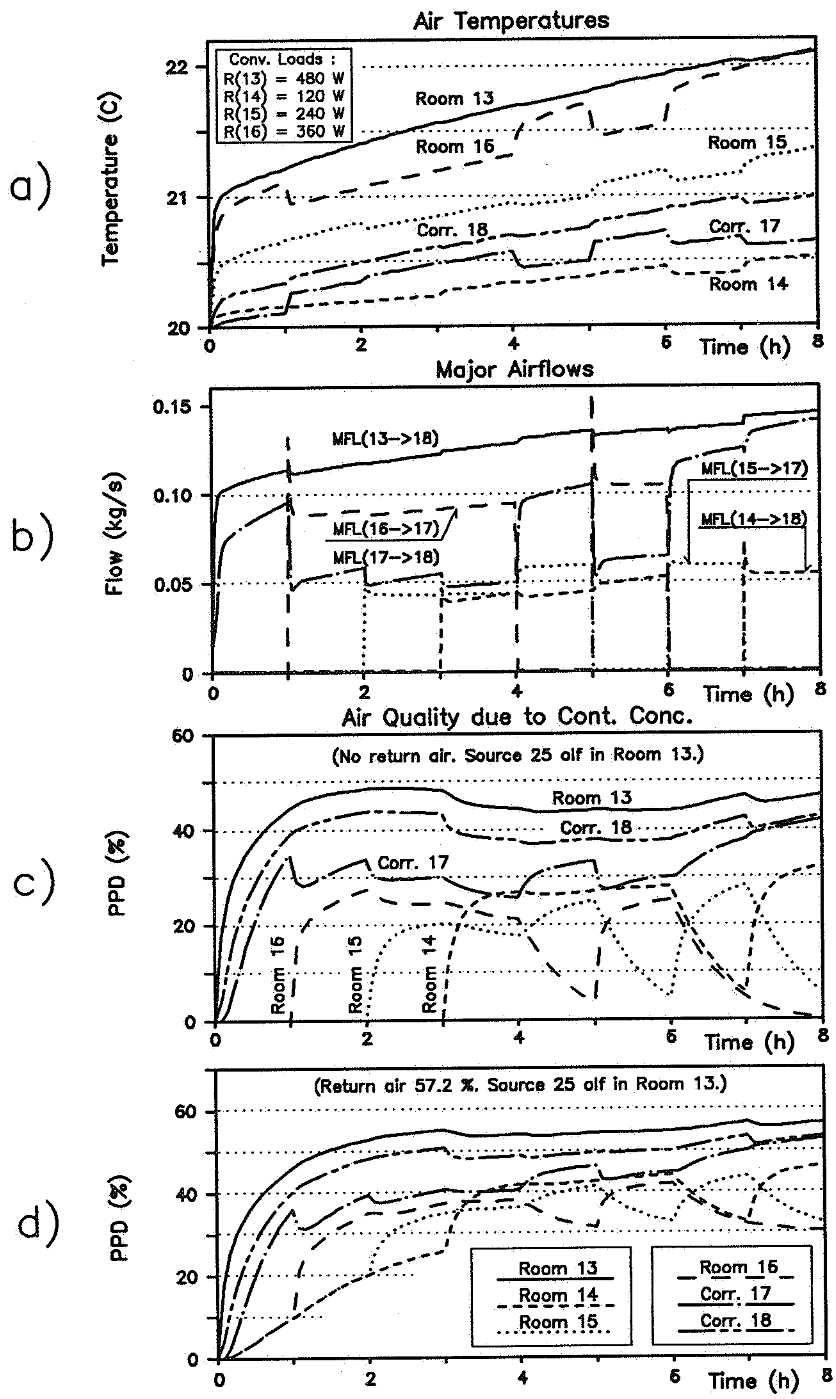


Figure 3. Air temperatures and air qualities in simulated building. All doors closed.

This generates a rapid increase in concentration in the room, since the concentrations in the corridoors are high due to the fact that the door of room 13 is open. Whereas very high concentrations, and thus low air qualities, are obtained within minutes of opening the door, it takes approx. 2 hours for the contaminant to be completely removed from the room after the door has been closed, see fig. 4c.

The use of return air attenuates the changes in concentrations imposed by changes in the position of the doors, evens out the distribution of concentration throughout the building and shifts all the concentrations to a higher level, see fig. 4d.



SCHEDULE								
D(13–18)	open	open	open	open	open	open	open	open
D(14–18)	closed	closed	closed	open	open	open	closed	open
D(15–17)	closed	closed	open	open	open	closed	open	closed
D(16–17)	closed	open	open	open	closed	open	closed	closed

Figure 4. Air temperatures, major airflows and air qualities in simulated building. Scheduled position of the doors.

7.3. Conclusions

The simulations showed that the air temperatures in a building do not remain constant, see figs. 3a and 4a. The phenomenon of two-way airflows through large openings is very sensitive to temperature, fig. 4b, and has a major influence on the contaminant transport from room to room. Thus the inclusion of thermal analysis in calculating contaminant concentrations considerably improved the reliability of the simulations.

The spread of contaminant in a building is affected by several factors and it seems to be difficult to protect a certain room from contaminant generated elsewhere in the system. Several conditions must be fulfilled to achieve it. First, the room must be maintained at a higher pressure than the rest of the system. Second, 100% fresh air ventilation must be used. Third, the door of the room must be kept closed. If any of the conditions is not fulfilled the contaminant will penetrate the room.

When air recirculation is used, the position of the door is of minor importance since the contaminant will find its way into the room through the air distribution system.
The door of the room where the contaminant is generated should be kept closed. This is the first measure to suppress the spread of contaminant to other spaces in the system.

8. SUMMARY

The computer program was developed for simultaneous dynamic simulation of contaminant concentrations, airflows and temperatures in multi-zone buildings. The theoretical foundations for the computer program were presented. A physical coupling was assumed as existing between the thermal behaviour of the building structure and the interzonal air movements. Thus its impact on the distribution of contaminants in the building was considered. This is a considerable improvement on other hitherto published programs in the same field.

An example building was used in a number of simulations. The dynamic distributions of contaminant concentrations in the building were determined with several door positions, with and without return air. The importance of simultaneous calculation of temperatures and airflows was evident, particularily in simulations including changes in the positions of doors.
The air qualities due to contaminant concentrations were evaluated in different parts of the building.

It was concluded that the first measure to suppress the spread of contaminant throughout the building is to keep the door of the room where it is generated closed. The airflows through the slots around the closed doors are unidirectional; therefore it is important to maintain rooms at a higher pressure than corridors. When the doors of the rooms are open, two-way flows through the door openings are established. The magnitude of two-way airflows through a large opening depends strongly on the temperature difference and is many times that of a one-way flow through a slot. Hence, the contaminant was efficiently distributed to all spaces when the doors were open. When air was recirculated, the contaminant penetrated all spaces in the system regardless of the position of the doors. Higher concentrations were obtained when the doors were open.

The basic simplification used in the program was the assumption of perfect mixing of air and contaminant within the zone. The thermal capacity of each partition in a building structure was roughly modelled as one value to be provided in input data. The outdoor air temperature was assumed to be equal at all outdoor nodes. The airflow through the large opening between vertically stacked spaces was simplified to a one-way flow.

The present version of the program works well and may readily be used for research purposes. Extensive validation by means of measurements should be carried out before it can be applied for design purposes.

APPENDIX

The following are the pressure-flow characteristics of nine types of airflow paths used in the program :

- Pressure loss in duct

$$\Delta p = 0.5 \, \rho \, v^2 \left(\frac{f_1 L}{D} + f_2 \right) \qquad (13)$$

where the pressure loss factor due to friction, f_1, is a function of duct diameter, roughness and Reynolds number.

- Power law for leakage equation

$$q = A \, (\Delta p)^B \qquad (14)$$

- **Quadratic leakage equation**

$$\Delta p = A\,q + B\,q^2 \qquad (15)$$

where coefficients A and B are constants and may be obtained from measurements [11].

- **Logarithmic element**

$$\Delta p = 10^A\,q^B \qquad (16)$$

where A and B are constants obtained from regression analysis.

- **Polynomial approximation**

$$\Delta p = s_0 + s_1 v + s_2 v^2 \qquad (17)$$

where coefficients s are constants.

- **Pressure loss across the damper**

$$\Delta p = 0.5 \cdot v^2 \cdot 2000 \cdot 10^{(e^{-A/4} - 0.0436\,A)} \qquad (18)$$

where A is the angle of the blades, (°); A=0° for closed damper and A=90° for fully open damper.

- **Pressure difference across the fan**

The velocity head generated by the fan is approximated by the second-degree polynomial

$$S_{ij} = s_0 + s_1 q + s_2 q^2 \qquad (19)$$

where q is the volume airflow (m^3/s), s_0, s_1, s_2 are constants and S_{ij} (Pa) is the velocity head. Equation (19) expresses the source term S_{ij} in eq. (4).

The general pressure loss coefficient K_{ij} for the path containing the fan refers to the pressure loss occurring in the part of the ducting included in the path.

- **Large opening between vertically adjacent spaces**

$$q = C_d A (2/\rho)^{0.5} (\Delta p)^B \qquad (20)$$

where C_d is the discharge coefficient.

- **Large opening between horizontally adjacent spaces**

$$q_{net} = 0.65 H W (2/\rho)^{0.5} (\Delta p)^B \qquad (21)$$

ACKNOWLEDGEMENT

This study was part of a project financed by the Ministry of Trade and Industry of Finland. This financial support is gratefully acknowledged.

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