An Integrated Approach to Indoor Contaminant Modeling

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ABSTRACT

Good indoor air quality is essential to ensure adequate internal environment conditions, avoiding possible problems related to health, productivity and comfort of individuals inhabiting a building. In order to appraise internal contaminant levels, taking into account sources, sinks and transport of pollutants from the outside and throughout a building, an indoor contaminant behaviour prediction method was developed using coupled thermal and massflow simulation. The developed approach was validated against analytical, inter-model and empirical results. It was shown that an integrated approach within a building performance simulation environment was necessary because situations exist in which assessment of just one domain does not give an accurate depiction of reality. This paper describes why it is important to take a global look at contaminant behaviour. It was found that significant errors could occur if spatial and temporal temperature variations are not included in the prediction of contaminant levels.

INTRODUCTION

Air pollutants are those chemicals that are not generally present in the atmosphere because of natural causes but are disseminated into the air by human activity. In most parts of Europe outdoor pollutants are principally the products of combustion from space heating, power generation, chemical industry waste or from motor vehicle traffic (McGinlay 1997). Indoor air environments contain a myriad of inorganic and organic gases and vapours typically in trace (parts-per-billion) quantities. The chemical composition of air varies widely between particular locations as well as between measurements taken at different times for the same location. The nature of these variations is such that it is difficult to definitively characterize a typical indoor air environment with respect to specific contaminants present and concentration levels (Kingsley 2000). A large number of air pollutants have known or suspected harmful effects that can be manifested on plant or animal life and / or the environment. Pollutants may not only prove a problem in the immediate vicinity of their emission but these can travel long distances and react with other species present in the atmosphere to produce secondary pollutants (Weschler 2004).

Major air pollution problems started after the Industrial Revolution as fossil fuels began to be adopted as the principal energy providers. What usually resulted were high levels of smoke and sulphur dioxide. The most perceptible after effect of this was smog. Smog, which is a health hazard in itself, can still be seen in many parts of the developing world (EPA 1999).

Indoor air quality (IAQ) is affected by transport of air and consequentially of pollutants from the outside. Many indoor activities e.g. cooking, smoking etc. contribute to indoor pollution. In addition, photochemical reactions resulting from the action of ultraviolet radiation on ozone (from photocopiers and printers) and on VOC (from outgassing of furnishings) leads to the formation of secondary long-range pollutants (McGinlay 1997). Radon emissions may be an issue of concern in some regions and unhealthy levels of humidity may cause persistent presence of dust mites and / or moulds.

The presence of contaminants -- intentional and unintentional – in the indoor environment causes problems in three general areas:

- Health problems
- Productivity problems
- Comfort and odour problems

It has been confirmed that contaminant and pollution problems are a factor in the so called Sick Building Syndrome (SBS). SBS is an umbrella term and some of the conditions manifested upon occupants, relevant to the scope of this document, are adverse skin, eye or pharynx symptoms, general headache or fatigue, lack of concentration, dizziness, general feeling of malaise, sleepiness, chills/fever, aching muscles, back pain, shoulder/neck pain, hand/wrist pain, problems with contact lenses, allergies, depression, seasonal affective disorder (Gyntelberg et al. 1994, Wallace et al. 1993, Hedge et al. 1995).

All of these symptoms have an impact on one or more of the previously listed problem areas i.e. health, productivity and comfort. The symptoms are experienced only after prolonged occupation of a particular building, i.e. daily or at least several times a week, and they disappear or are significantly reduced minutes or hours after leaving the building (Gyntelberg et al. 1994). Poor IAQ is the cause of excessive morbidity and mortality. In developing countries unvented burning of biomass for cooking is the cause of at least 2 million deaths a year (mainly women and children) (Sundell 2004), and in the developed world poor IAQ is a main cause of allergies, other hypersensitive reactions, airway infections and cancers. A crude estimate of the magnitude of productivity gains that may be obtained by providing better indoor environments for the U.S. alone stands at $6-19 billion from reduced respiratory disease, $1-4 billion from reduced allergies and asthma, $10-20 billion from reduced SBS symptoms and $12-125 billion from direct improvements in worker performance that are unrelated to health. Sample calculations indicate that the potential financial benefits of improving indoor environments exceed costs by a factor of around 250% (Fisk et al. 1997).

There has been a shift of interest in the whole conceptualisation of indoor human comfort in recent times. Focus seems to have shifted from thermal satisfaction and odour prevention to health related and productivity issues (Samet 1993). In brief, there is a lot of interest in the specific area of health issues related to the indoor environment and a large amount of work is currently being done in this research field. To study this it is important that contaminant prediction be integrated within whole building simulation and appraised along with other 'conventional' metrics.

INTEGRATED SIMULATION

From the point of view of the present work, previous research studies have shown that not taking into account dynamic temperature differences has a considerable impact on predicted air flows and contaminant transport (Bossaer et al. 1999). Work reported in this paper confirms this finding. This brings in question the relevance and reliability of standalone airflow prediction tools. Although some work has been reported on linking contaminant prediction into thermal modelling (Weber et al. 2003) no applications have been presented.

Buildings and related energy systems can easily have tens of principal parameters (insulation level, capacity position, ventilation rate, glazing area, glazing type, lighting load, fuel type and so on) and the permutations available for the domain configuration are very large (SESG 1999). Within ESP-r (Clarke 2001) a building comprises a collection of mutually interacting principally thermodynamic domains. Each domain is solved by the specific nature of its underlying theory (linear/non-linear, sparse/compact, iterative/non-iterative etc.). These domains are integrated with each other to emulate the real time behaviour of a building. Examples of some important couplings are building thermal processes/natural illuminance distribution, building/plant thermal processes/distributed fluid flow, building thermal processes/intra room air movement, building distributed air flow/intra room air movement, electrical demand/embedded power systems (renewable energy or otherwise), construction heat, moisture flow. These domains interact in a nontrivial manner. To determine the state of such a large number of domains requires integrated simulation of all the systems simultaneously.

Two approaches can be adopted to integrate the different domains: internal coupling and external coupling. Djunaedy et al. (2003) discussed different approaches to coupling two programs. Internal coupling can be seen as a form of program extension and essentially expands the capabilities of existing software by adding new modules into an existing program. External coupling on the other hand makes use of existing packages in different domains (for example thermal building simulation for the thermal domain and CFD for the flow domain) and provides a mechanism for these programs to communicate. External coupling is defined as a runtime communication of two separate programs (or modules within the same executable) where at least one of the programs (or modules) continues to run while exchanging information with the other program (or module). External coupling has at least two major advantages over internal coupling. Firstly each domain application has evolved separately over the years and is well proven. Rewriting the code to be included as part of another package could be seen as a setback from these independent advances in separate domains. Therefore further efforts would better be concentrated at making these different domain applications communicate with each other. Secondly external coupling can immediately benefit from independent developments in each domain. The separate domain applications can expand and develop in their respective directions, and the external coupling mechanism can make this development available without having to update the source code appreciably (Djunaedy et al. 2005).

External coupling can either be sequential or simultaneous. In the sequential approach the first module solves, results from it are input into the second module, then the second module solves and simulation progresses to the next time step. In the simultaneous approach the two domains keep on passing information back and forth until some mutual convergence criterion is satisfied. The simultaneous approach can thus be much more computationally intensive, but it has been shown to be more accurate than the sequential approach for certain building designs (Hensen 1995).

ESP-r is especially suited to coupling within itself because of its modular nature and because much of the common information between two domains need not be written out twice. Information would need to be written twice (i.e. once in each tool) for the case of two unique simulation tools. Two otherwise independent ESP-r modules can write to and read from the same FORTRAN common block (which is just a collection of variables with some unique names) and this can thus provide a mechanism of communication. Communication between two independent tools would have to take place at a system level i.e. external to the tools themselves.

For the present coupling approach of airflow prediction and building thermal simulation it is thought that this work will be of importance in better modelling of configurations that depend solely or heavily on temperature dependent flow. Configurations such as purely natural ventilation schemes and mixed mode ventilation schemes could be ideal candidates. Although flows dominated by mechanical ventilation or wind induced pressure are not so dependent on temperature, integrated modelling can still be important in order to determine heating and cooling loads. The case study presented in this paper is chiefly mechanically driven flow but it serves to demonstrate domain interaction.

CONTAMINANT SIMULATION

The state of the art in standalone contaminant simulation tools may be divided into two categories:

- Network model based
- CFD based

The network based tools first solve a mass flow nodal network (Hensen 1991, Walton 1988) and then compute contaminant concentrations for mass flow nodes. The contaminant analysis may be based (employing contaminant mass conservation) on simultaneous solution of contaminant flow equations. Temperature may be defined via schedules. An example of this type of tool is CONTAM (Dols and Walton 2002). CFD based tools employ mass, momentum and energy conservation principles to obtain among other results, micro-climatic contaminant concentrations. An example of such a tool is FLUENT (FLUENT 2003).

The approach described in this paper is similar to the former but, instead of using fixed temperatures, a fully integrated approach is adopted. Contaminant concentrations are still post-processed after running the mass flow solver but by including other building performance domains such as lighting, thermal and plant domains for the mass flow solution, simulation results will take into account these interactions and hence be more representative of reality.

The contaminant transport model assumes that the ambient contaminant concentration is known and that the mass of contaminant transported indoors / outdoors is a function of the air massflow rate obtained from the network airflow model. Hence the contaminant massflows are in effect directly proportional to the air massflow rates. Contaminant concentrations are solved simultaneously using a Crank-Nicolson scheme by default.

THEORETICAL MODEL

The contaminant simulation model is intended to take into account:

- Contaminant transport
- Generation and decay within a zone
- Filter efficiencies for the different flow paths
- Ventilation control based on concentration of a particular contaminant
- Simulation of first order chemical reactions

Much of this model is based on the CONTAM (Dols and Walton 2002, Walton and Dols 2003) model, but conflation within the whole building simulation environment, ESP-r, enhances contaminant modelling to include effects from aforementioned building thermodynamic domains on airflow and consequently contaminant transport.

In matrix form, transient contaminant concentration can be given by:

$$Q^* = Q + Q^{\circ}\Delta T \qquad (1)$$

where Q° is given by:

$$Q^{\circ} = KX + S \qquad (2)$$

The air mass flow rate matrix K has on its principal diagonal the total mass flowing out from an internal node. The other elements in the matrix are flows to other nodes and chemical reaction rate constants. The matrix is of order number of nodes times number of contaminants. The matrix elements are filled following the four rules below:

$K_{ij} = -\sum m_n$ $[i=j]$

$[N(n-1)+1 \leqslant i \leqslant Nn]$

$K_{ij} = k$ $[i \neq j]$

$[N(n-1)<j \leqslant Nn]$

$[N(n-1)<i \leqslant Nn]$

$K_{ij} = m_{ln}$ $[i \neq j]$

$[j=N(l-1)+\tilde{N}]$

$K_{ij} = 0$ $[i \neq j]$

$[j \neq N(l-1)+\tilde{N}]$

In the above equations N is the total number of contaminants and n goes from 1 to the total number of nodes in the system. A weighting factor ζ is then established for equation (1) to average present and future timerow values (the default value is taken to be half, the Crank-Nicolson scheme which provides unconditional stability):

$$Q^* = Q + (1 - \zeta)\, Q^{\circ}\Delta T + \zeta Q^{\circ *}\Delta T \qquad (3)$$

Equation (2) in its current state contains 'known' values in the airflow matrix K. These known values originate from taking into account all nodes of the airflow network. Some of these are boundary nodes and because contaminant concentrations would have been initialised to ambient values, these should be removed before soultion. In order to do this Q° was redefined as follows:

$$Q^{\circ} = KX + V + S \qquad (4)$$

The effect of known concentration nodes is accommodated by the vector V, and corresponding rows in matrix K are initialised to zero. K is then preconditioned to remove these rows before calculation. This preconditioning also removes rows associated with unconnected internal nodes.

The contaminant mass vector Q can be defined as the product of air mass and contaminant concentration for a node. In matrix notation it is equivalent to:

$$Q = MX \qquad (5)$$

Putting equations (4) and (5) in (3) gives the following relation:

$$(M - \zeta K\Delta T)X^* = MX + \Delta T\{(1 - \zeta)\, KX + V + S\} \qquad (6)$$

This equation is solved for X* using Gaussian Elimination with backsubstitution and no pivoting. The matrix $(M - \zeta K\Delta T)^{-1}$ is forward reduced halfway, to a matrix with components on the diagonal and above remaining nonzero. The solution vector X* is then generated through backsubstitution of the known right hand side vector.

Major Limitations and Assumptions

The contaminant simulation model is based on calculation of concentrations assumed from mass conservation of contaminants. Contaminants are assumed to be fully mixed within the air and therefore contaminant transport is directly proportional to air flow between nodes. The airflow network solves first and the airflows are then used to calculate contaminant flow. The contaminant model thus can at best be as accurate as the airflow network model it is based on and all assumptions used for solution of the air flow network are implied for the contaminant model. The airflow network model is well established and understood. There is much documentation available (Lorenzetti 2002a, Hensen 1991, Walton 1988) and exhaustive explanation of assumptions have been reviewed. Some of the principal assumptions and limitations in this model as implemented are given below.

Assumptions regarding air flow network:

- Mass flow is a function of pressure difference only.
- Each node connects directly or indirectly to a boundary pressure node.
- Pressure and density of air at a node are taken to be a single value.
- Mass flow always increases and never decreases if the pressure difference increases.

Assumptions regarding contaminant prediction model:

- There are no contaminant transportation delays; therefore in some cases propagation rate of contaminants may be overestimated or underestimated for poorly mixed zones.
- Particulate matter is treated just like gas, and there is no mechanism to address processes like deposition (possibly gravitational settling), coagulation, etc.
- Contaminants are considered to be 'trace' i.e. they do not affect the density of air and have negligible partial pressure.
- Air and contaminants in a thermal zone are fully mixed so intra-zone contaminant distribution cannot be appraised.

Probably the most important decision for a suitable solution method is that components are restricted to produce a symmetric Jacobian matrix. At each time step, *mfs* (the ESP-r network mass flow solver) repeatedly calculates and factors new Jacobian matrices. During this process it extracts trial solutions for the network using the Newton-Raphson method. A symmetric matrix requires only about half the storage capacity and may be factored in about half the time as a full matrix (Dennis and Schnabel 1996). The solution mechanism is accelerated within *mfs* by adopting an approach similar to Steffenson iteration (Clarke 2001). The efficiency gains are important because matrix factorisation dominates the solution time for the non-linear system. Another characteristic of this Jacobian matrix is that it is positive definite; this property guarantees existence of a unique solution (Lorenzetti 2002a). One assumption this leads to is that flow rate increases with pressure difference so as to ensure a positive rate of change. Another assumption is that each node connects directly or indirectly to a boundary node. Most flow components satisfy the first criterion. The second requirement is a function of mass flow network topology rather than flow components (Lorenzetti 2002b).

The flow network approach does not incorporate momentum because a steady state flow based on pressure differences is calculated. Another potential problem could be delays associated with pollutant transport in flow paths. Dealing with this aspect would require accounting for both the pollutant mass stored in the flow paths and the time needed to carry it between nodes. Modelling all transport as instantaneous simplifies the assembly of the defining equations, but over-predicts the speed at which pollutant spreads through the building.

VALIDATION

Validation of the contaminant processing implementation was undertaken by first defining the validation methodology. Different validation exercises are then detailed. The PASSYS validation methodology (Jensen 1993) was adopted. It was produced by the Commission of the European Communities PASSYS project and includes all stages of simulation program validation. The methodology comprises five components, not all of which need to be applied in a given context:

- Theory checking: theory of the developed computer model is examined to confirm that the theory is appropriate in terms of its application and scope.
- Source code inspection: the code should be checked to ensure that the selected algorithms are correctly implemented.
- Analytical verification: output of the whole package or part of it is compared with the analytical solution for relatively simple contaminant distribution problems.
- Inter-model comparisons: calculated results from the developed scheme are compared with other schemes within the program itself, or other programs which are considered to be better validated.
- Empirical validation: the output of the program is compared with monitored results from a real structure such as test cells.

Theory for the model was compared against mathematical models to ensure applicability was within the scope of contaminant modelling. Structured programming and documentation ease the process of source code examination. Code checking tools (for syntax errors) and debugging tools (for logic errors) were used.

Analytical Validation

For the purpose of analytical validation a number of hypothetical test cells were created within ESP-r and contaminant simulation run against steady state weather conditions to obtain contaminant concentration values. The results were then compared against analytical solutions.

The first test comprised a simple one room model with three airflow nodes (two boundary and one internal). Constant ambient concentration of 4.6×10^{-4} kg/kg CO_2 was assumed and the variation of interior concentration with time was compared against analytical calculations. Less than 0.1% error in predicted concentration was obtained for this test.

Figure 1 shows details for test 2. (For simplicity exhaust fans and node 3 were not included in the analytical validation but retained for inter-model validation). The simulation time step used was 5 minutes. The contaminant chosen was water vapour, which can be modelled as a contaminant. An external concentration of 0.002173kg/kg was chosen; this corresponds to a relative humidity of 50% at 2^0C (35.6^0F) and 1.01325 bar atmospheric pressure (Rogers and Mayhew 1995). Results for this test for node 2 are shown in figure 2. Results show good agreement for all the nodes between the ESP-r contaminant model and the following analytical solutions:

$$C_2 = C_{amb}(1-e^{-k_2 t}) \quad (7)$$

$$C_5 = C_{amb}(1-e^{-k_5 t}(1+k_5 t)) \quad (8)$$

$$C_6 = C_{amb}(1-e^{-k_6 t}(1+k_6 t+\frac{k_6^2 t^2}{2})) \quad (9)$$

Here *k* is defined as the node decay constant given by (total air mass flow rate into node)÷(mass of air in room represented by the node).

Convergence Checking

Convergence criteria are defined by Versteeg and Malalasekera (1995). In test 3 it was ascertained whether the numerical solution converged to the analytical solution as the timestep was reduced. It was found that as the time step was decreased from 10 minutes to 1 minute the error in concentration compared to the analytical solution decreased and there was rapid convergence to the analytical solution (figure 3).

Inter-model Validation

The model considered for inter-model validation was similar to the one used for test 2 and is shown in figure 1. A steady state climate of 20^0C (68^0F) dry bulb temperature and zero wind speed was chosen. Similar models were built using CONTAM and ESP-r and compared. It was also possible to use analytical results in this validation study.

There were three permutations of a basic model:

- Test 4-1: Two contaminants *contaminant1* and *contaminant2* were considered; both had ambient concentrations of 0.0008kg/kg. Initial concentration of *contaminant1* was zero in all three zones but *contaminant2* had an initial concentration of 0.0020, 0.0016 and 0.0012kg/kg in zones *room3*, *room1* and *room2* respectively.
- Test 4-2: Similar to test 4-1 but with the addition of a source of 0.005kg/s (0.011lb/s) in zone *room1* and a source of 0.005kg/s (0.011lb/s) in *room2* with a cutoff concentration of 0.2kg/kg. Contaminant generation from the source is assumed to decrease as its concentration in the air increases until the source stops emitting any more contaminant when the concentration reaches a critical or cutoff value. Both sources were for *contaminant1*.
- Test 4-3: Similar to test 4-2 but with an addition of a filter efficiency of 13% for air entering node two.

Results for test 4-1 are shown in figure 4; results from the other two tests were similar in trend. The results from the two models were compared based on ASTM guide D5157-97 Standard Guide for Statistical Evaluation of Indoor Air Quality Models (ASTM 2003). This standard provides information about statistical tools for assessing model performance. The standard gives three statistical metrics for assessing accuracy and two additional metrics for assessing bias. Statistical evaluation of the different parameters based on the ASTM guide show that the results from CONTAM and ESP-r are within a small tolerance (1%) of the analytical solution and fulfil the various ASTM D5157 criteria. It should be noted though that the guide is for the combined comparison of both airflow and contaminant predictions whereas for the purpose of this study the airflows were maintained at uniform levels in the models by use of constant flow rate components.

Empirical Validation

Results of a previously conducted study (Bossaer et al. 1999) were used. This comprised an evaluation of a COMIS (Feustal and Smith, 1997) model by experimental comparison. The ESP-r model was built according to the COMIS model and the spread of contaminant in the built space was studied.

The model consists of a flat in a suburban area near Namur in Belgium. The building has nine storeys, each with four apartments. Measurements had been made in a unoccupied flat on the ground floor. Figure 5 shows the plan of the flat as built in ESP-r. It consists of seven zones: *LIV* (living room), *KIT* (kitchen), *BED1*, *BED2* (bedrooms), *HALL*, *BATH* (bathroom) and *TOIL* (toilet). The airflows into the apartment are from *LIV*, *BED1*, *BED2*, *HALL* and *KIT*. Air flows out of the apartment via ducts from *KIT*, *BATH* and *TOIL*.

The airflow network as modelled in ESP-r is shown in figure 5. Contaminant (CO_2) was injected into *BED2* at the rate of 14ml/s (0.854cu. inch/s) for two hours and the concentrations of the gas were simultaneously measured in *BED2* and all other zones. Measurements were performed at several places within one zone and the results averaged. This was thought to be representative of the concentration of CO_2 in that zone. Flows due to wind were measured in the original study by tracer gas techniques and the measured flow rates imposed on the forced flow components in the model. Components used included:

1. Door components to model bi-directional flow. The dimensions of the door were 0.85m (2.79ft) by 2m (6.56ft) and the coefficient of discharge was 0.6.
2. Cracks to model the exit of air from *KIT*, *BATH* and *TOIL*. The crack dimensions in the original study could not be determined and a number of simulations were carried out to determine how the final results were affected by it. There appeared to be a large deviation when choosing different crack dimensions. Results for typical crack dimensions that gave reasonable correlation for the experimentally determined airflows are reported.
3. Forced airflow components with known flow rates were used to model wind effect on the different inlets. The flow rates changed over time and average flow rate per hour was used.

For the purpose of simulation the wind effect had already been taken into account; therefore a climate file with zero wind speed was used. The original study reported that temperature differences within the different rooms was a major contributor to the associated airflows and therefore to the concentrations of contaminant therein. The temperature was carefully controlled to the nearest 0.1^0C (0.18^0F). It was confirmed in the present work that temperature differences did indeed contribute remarkably to the airflow. Simulated flow rates as large as 40% different from measured flow rates were obtained before the measured temperatures were incorporated into the model.

The model was simulated using ESP-r. Contaminant injection was modelled by a uniform source term for *BED2* that came on during the two hours of injection. Results were obtained for the concentration of CO_2 in the various zones. Figure 6 shows transient concentrations of the contaminant in two zones. There is a fair degree of agreement between COMIS, ESP-r and the experimental observations. Results were checked based on ASTM D5157 and findings for two zones are recorded in table 1. It can be seen that both COMIS and ESP-r do not fully satisfy ASTM D5157-97 criteria. For *BED1* the NMSE is outwith prescribed results, and for *BED2* the regression line intercept (*a*) differs for ESP-r.

TABLE 1

ASTM D5157 criteria for two zones for Namur flat[1]

	BED1		ASTM D5157 prescribed results
	COMIS	**ESP-r**	
r	0.97	0.98	0.9 or more
a	-96	-53	±52 or less
b	1.51	1.08	0.75 to 1.25
NMSE	0.83	0.44	0.25 or less
FB	0.05	-0.20	0.25 or less
FS	0.20	0.09	0.5 or less

[1] The various D5157 parameters are defined as:

r = correlation coefficient
b = slope of line of regression
a = intercept of line of regression
NMSE = normalized mean square error
FB = fractional bias
` FS = similar index of bias

	BED2		ASTM D5157 prescribed results
	COMIS	ESP-r	
r	0.99	0.99	0.9 or more
a	29	-120	±108 or less
b	1.29	1.25	0.75 to 1.25
NMSE	0.14	0.21	0.25 or less
FB	0.31	-0.03	0.25 or less
FS	0.53	0.46	0.5 or less

This tends to suggest that the measured and predicted concentrations differ significantly but correlation between these concentrations is high as can be seen by the high value of correlation coefficient (*r*). Nevertheless the results do show that the integrated ESP-r contaminant model shows appreciably close agreement with COMIS predictions and empirical data. There are some important factors to consider before drawing conclusions as to COMIS and ESP-r modelling capability from this test. Emmerich and Nabringer (2001) discussed that an absolute validation of a complex building thermal and airflow model is impossible, because the user can create an infinite variety of models. However one important reason to perform experimental validation is to identify and hopefully eliminate large errors (Emmerich and Nabringer 2003). For the situations modelled in this effort no large errors in the ESP-r model were identified.

Additionally it must be understood that the experimental model was subject to its own uncertainties and imprecisions. These are much more than precision limits of measurement devices. While there is no doubt that within the original study every effort was made to obtain accurate results, the placement and orientation of sensors, injection and measurement points of tracer gas would all have a bearing on the final answer. The model while being quite detailed, could have been improved. Specifically it would have been beneficial to have known crack parameters and not make educated guesses. It should be stressed here that the ASTM D5157 guide is just a guideline, not the final judge of model accuracy. Rather than the specific parameters and criteria, its primary value may be to move model validation beyond the oversimplified analysis of simple differences and percentages and towards useful statistical analysis of model validation results (Emmerich and Nabringer 2003).

CASE STUDY – Public House in England

Figure 7 shows a public house in England which was studied to show how CO_2 and CO from smoking varied within occupied hours. The model consists of five zones named *public*, *lounge*, *bar*, *conser* and *conser_sun*. The model was built to study thermally induced effects on the air flow (and hence on the contaminants transfer) of a new conservatory that was to be built on the south side of the public house. This conservatory was modelled by the two zones *conser* and *conser_sun*. This study also investigated the opposing demands made by the requirement of provision of adequate air quality and the requirement of provision of adequate thermal comfort on the HVAC system. As a worst case scenario simulations were carried out in winter in order to exacerbate the contrast between energy provision for heating and IAQ. This was hoped to provide information that might lead to understanding of the important point that increasing ventilation rate provides better IAQ but increases energy demands for heating at the same time. Furthermore one section of the building (the public bar represented as zone *public*) was designed to be a smoking area, hence aggravating the problem of providing adequate indoor air quality.

Design air temperature for the winter time was 21^0C for all parts of the building except the zone *bar* which had a design air temperature of 18^0C(64.4^0F). The occupancy was modelled as 160 people between 1200-1400 and again between 1900-2400. Between the hours 1400-1900 it was assumed that the building operated with reduced occupancy of 32 people. This occupancy was divided among the various zones comprising the building in rough proportion to floor areas so as to give an even (and realistic) spread of occupant casual gains and CO_2 emissions. Occupants were assumed to be the only sources of CO_2. The occupants were further assumed to be generating heat at the rate of 140W per person. This metabolic rate corresponds to 5.6×10^{-3} l/s (0.342cu. inch/s) of CO_2 (Liddament 2004). Ambient concentration of CO_2 was assumed to be constant at 4.6×10^{-4} kg/kg. Occupant smoking was modelled using carbon monoxide CO. Although tobacco smoke contains numerous chemicals only one is modelled in order to simplify the problem; furthermore it is assumed that the path taken by one chemical from tobacco smoke will be similar to the path taken by other chemicals of the same origin. The amount of CO given out from one cigarette is 58.5mg (0.00206oz) (ARBSSD 2005). It was assumed that 75% of occupants in the smoking area were smoking at any given time and that one cigarette lasted 5 minutes.

Figure 8 shows model detail where a plan view and south elevation of the building divided up into thermal zones is drawn. The bulk of the simulated space is the occupied space which can be divided up into three principal regions: the public space where the main entrance is located which is also the smoking area within the building, the zone *lounge* which is a non smoking space which also has an entrance and is similar in occupancy patterns to the public bar and the conservatory which is a non-smoking space. The south eastern section of the conservatory is the conservatory proper i.e. with most of the wall area comprising transparent construction. For this reason it is modelled as a separate thermal zone *(conser_sun)*. The simulated space consists of around $250m^2$ (2700 sq. ft) of floor area occupying a space of more than $1000m^3$ (35000cu. ft). Built with typical construction materials the public house has brick walls with glass wool and air insulation for walls. The roof is light mix concrete with roofing felt, glass wool insulation and plaster board finish. The floor is common earth packed and gravel based with heavy mix concrete followed by glass wool insulation, chipboard and carpet.

A detailed air flow model comprising five internal, two ventilation system and fourteen external nodes was built to describe various forced and unforced air flows. This is shown in figure 9. A balanced HVAC system was used to define intentional air flows for the building. Fresh air is introduced in the region above the bar i.e. in the thermal zone called *bar*. This air is then assumed to flow to the public and lounge spaces. Additional ventilation air inlets are provided in the zone *conser*. Air is extracted from *public*, *lounge* and *conser*. Airflows between the zones were modelled using door type air flow components that allowed bi-directional flow. Unintentional flows through small openings around windows and other openings to the ambient were modelled using crack type components. Effort was made to account for all flow paths in the building. Ventilation rate for the building was taken to be at 8l/s per person and this was maintained even when the building was operating at less than design occupancy. Heating was achieved by heat input directly to the room and all fresh incoming air was considered to be at ambient temperature. This model supplied an opportunity to study the effects of providing enough air for dilution of contaminants against space heating energy requirements.

Detailed simulations are presented for one winter day i.e. 8^{th} January. CO_2 is used as an indicator for indoor air quality because of its relative inertness in the indoor environment, homogeneity and ease of measurement. The ventilation system was designed to maintain a lower pressure in the smoking parts of the building (thermal zone *public*); this in turn could cause CO_2 to accumulate there. CO is used as an indicative contaminant that indicated how the contaminants generated by smoking would be distributed.

Flow control was also defined in the model. The windows in the model were opened when the CO_2 levels in that zone were above some threshold value. An alternative thermal control was also defined in which case windows were opened when temperature in the zone rose above some threshold value. At any given time either contaminant based control or temperature based control could be employed.

Results and Discussion

The first control strategy attempted was temperature based i.e. heating came on when temperature dropped below the thermostatic setpoint of 20^0C. Furthermore, ventilation was assumed to operate at 100% during occupied hours (1200-2400). It was found that with this control strategy the heating requirements for all spaces was 540kWh for the occupied period. This gave high CO_2 concentrations in some parts of the building. Concentrations for each zone are shown in figure 10. It can be seen that concentration in most parts of the building is relatively low except the zone *conser_sun* which does not have any extract. It can be stated that all zones show poor air quality in terms of contaminant concentration because the generally accepted level of CO_2 is around 1000ppm or 1.0g/kg (Sundell 1982).

The second control option studied can be called occupancy based control (i.e. ventilation was adjusted in proportion to occupancy and temperature based heating control as before). It was assumed that occupancy would be reduced to 20% in the quieter afternoon hours of 1400-1900. Correspondingly, ventilation rates were lowered to 20% during that time. It was found that although the heating energy requirement dropped by about 50% to 274kWh, CO_2 concentration rose dramatically in all zones. Zone concentrations are shown in figure 11. If this was a study of just space heating requirements and energy efficiency such a control may have been reported as a possible solution.

The maximum concentration was approximately 4500ppm in the zone *conser* for this type of ventilation control. The levels obtained were considered to be high but can be corroborated using experimental studies (Carrer and Maroni 2002, Corsi et al. 2002, Sowa 2002). To get a better picture this simulation was repeated a number of times with increased ventilation up to a maximum of 600%. Figure 12 shows heating energy results from the various simulations and maximum CO_2 concentration. It can be seen that acceptable contaminant levels and hence adequate indoor air quality can be provided with six times the recommended ventilation level.

Being able to provide suitable air quality with 600% recommended ventilation plant size and more than four times more energy is clearly not the optimal solution. Problems in the original design and implemented control was then sought and possible solutions explored. One of the obvious problems with the ventilation system was improper air extraction from the zone *conser*. The air introduced in that zone was based on the combined load of that zone and *conser_sun* but there was no mechanism for extract from *conser_sun*. Extract was therefore redirected via zone *conser_sun* instead of zone *conser*. This improved both energy requirements and contaminant concentration. It was found that restricting CO_2 levels to slightly more than 1000ppm could be achieved by increasing ventilation by a factor of 2 and using contaminant based ventilation control. This corresponded with a heating energy requirement of 880kWh.

CO tracking for the building shows that the zone *public* has highest concentration as expected but the ventilation system seems to be providing adequate ventilation air and the maximum concentration is 220ppm. Although there is no safe level for CO this concentration is below typical concentrations within smoking spaces

(ARBSSD 2005). Figure 13 shows CO variation for the different zones for the ventilation scheme with extract from the zone *conser_sun*.

CONCLUSIONS

An approach to contaminant modelling that is integrated with other domains of building simulation is presented. Literature review suggests that there are some configurations (especially natural ventilation and stack driven flow regimes) in which knowledge of transient temperature distribution is important to correctly predict air flows and hence contaminant concentrations. Currently implemented theory is quite similar to CONTAM but contaminant simulation takes place after an integrated massflow solver has run. It thus takes into account transient temperature fields and does not depend on pre-simulation defined schedules.

The work done in this research of integrating contaminant prediction and thermally integrated air flow modelling has made it possible to study contaminant behaviour and transport within the built space with a greater accuracy than by using standalone (i.e. not thermally coupled) network air flow and contaminant prediction tools. This is because temperatures are predicted dynamically and the program does not rely on predefined schedules. Consequentially air flow rates between the different areas of a building are more realistic and so are the contaminant flow rates which depend on air flow rates.

After integrating the contaminant model within the whole building simulation environment ESP-r, validation studies were conducted. The bulk of this comprised analytical, intermodel and empirical comparisons. ASTM D5157-97(2003) criteria were also investigated for the model and in most cases were found to be satisfied.

A case study using the newly developed contaminant transport and distribution model showed that with typical ventilation and air supply regimes it is possible that contaminant levels rise significantly (adequate thermal comfort being provided). This case study provides an illustration of how indoor air quality can be compromised because of energy conservation considerations. It is not meant to understate the importance of good energy economy and efficiency measures but to imply that good air quality is also an important issue to consider when appraising energy conservation measures. Furthermore good design of a ventilation system can lower energy requirements for a space and at the same time alleviate poor air quality problems. It was found that with an energy overhead of 60% CO_2 levels fell from 4500ppm to little above 1000ppm.

NOMENCLATURE

(Italics refer to symbols used in analytical solutions)

$C_{\alpha n}$	Concentration of contaminant α at node n (kg/kg)
$C_{\alpha amb}$	Ambient concentration of contaminant α (kg/kg)
K	Air mass flow rate matrix (kg/s)
k	Node decay constant (s^{-1})
K_{ij}	Elements of air mass flow rate matrix (kg/s)
k	Reaction rate constant for contaminants (s^{-1})
M	Zone air mass matrix (kg)
m_n	Total air mass flow out of node n (kg)
m_{nl}	Air mass flow from node n to l (kg)
N	Total number of contaminants
Ñ	Contaminant number
n,l	Nodes of interest
Q	Contaminant mass vector (kg)
Q°	Contaminant mass flow rate vector (kg/s)
$Q^{\circ}*$	Future time row contaminant mass flow rate vector (kg/s)
Q*	Future time row contaminant mass vector (kg)
S	Contaminant source / sink rate (kg/s)
t	Time (s)
V	Contaminant mass flow rate from ambient nodes vector (kg/s)
X	Contaminant concentration vector (kg/kg)
X*	Future time row contaminant concentration vector (kg/kg)
ζ	Weighting factor (-)
α	Contaminant identity (-)

ΔT Timestep (s)

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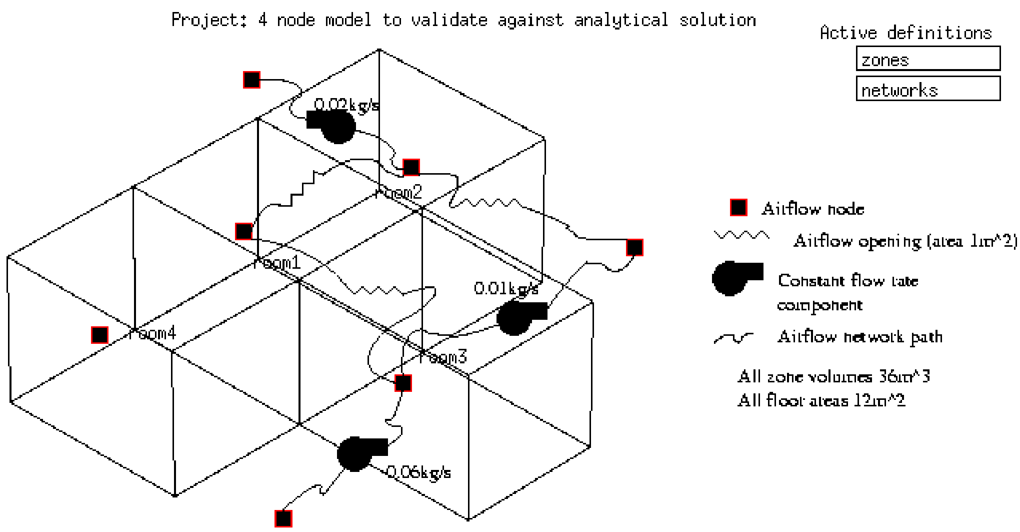


Figure 1 Project model and test cell for analytical and inter-model test

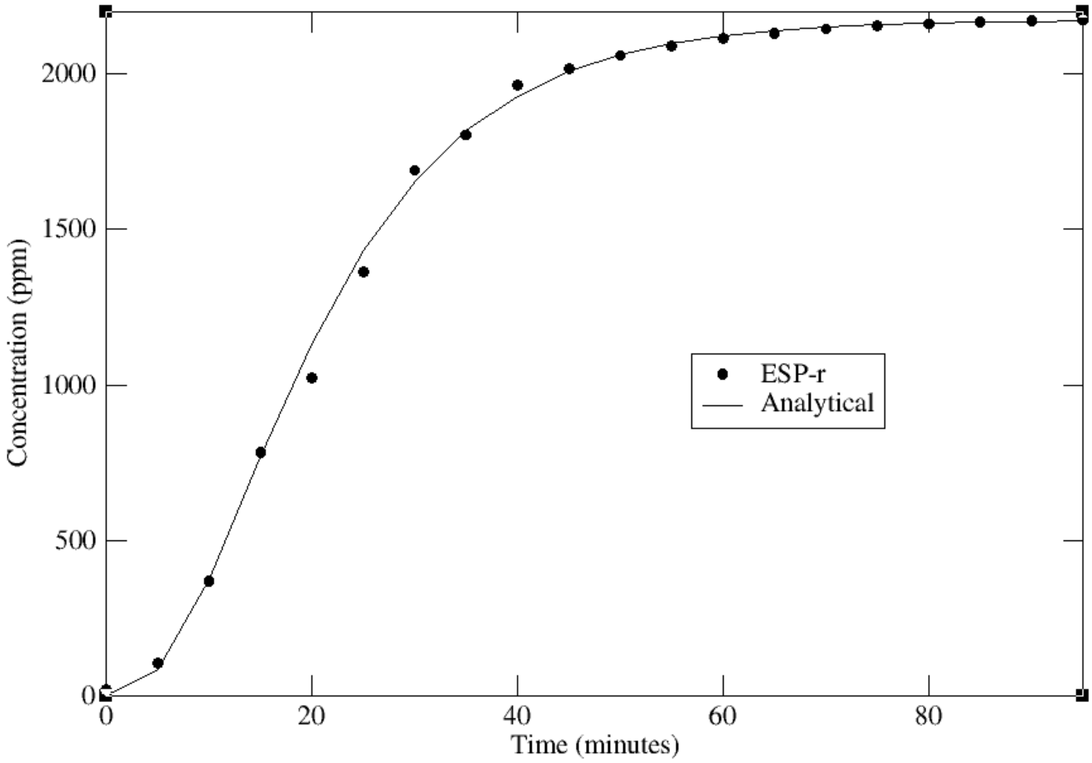


Figure 2 ESP-r and analytical results for node 2 in test 2

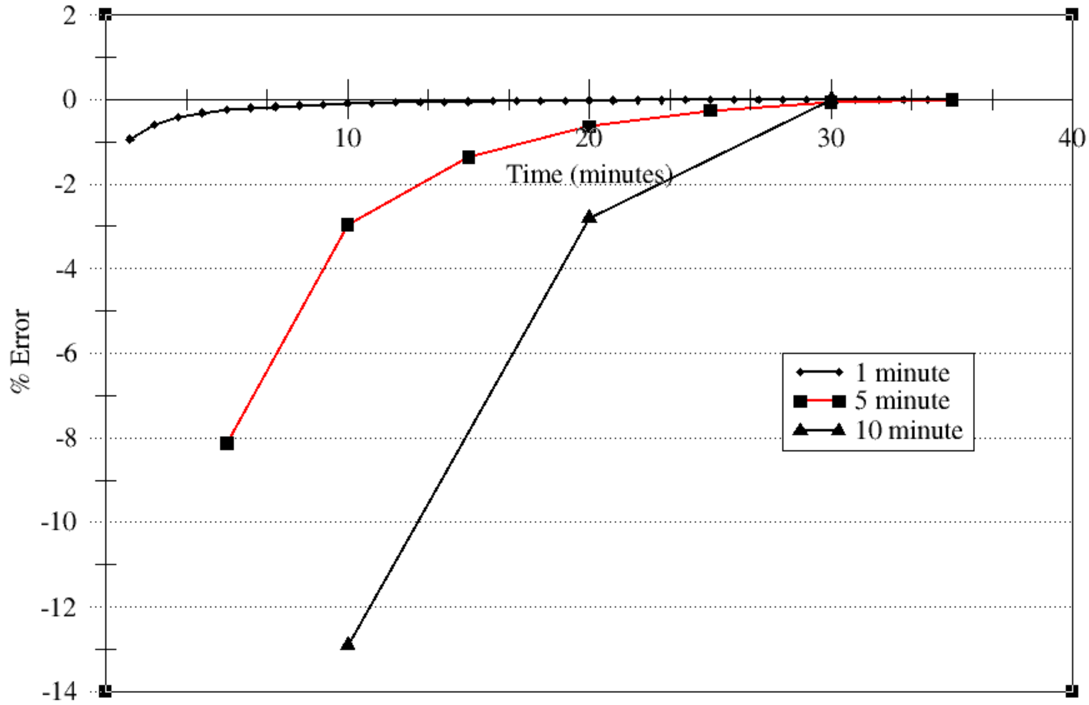


Figure 3 Effect on accuracy of reducing time step

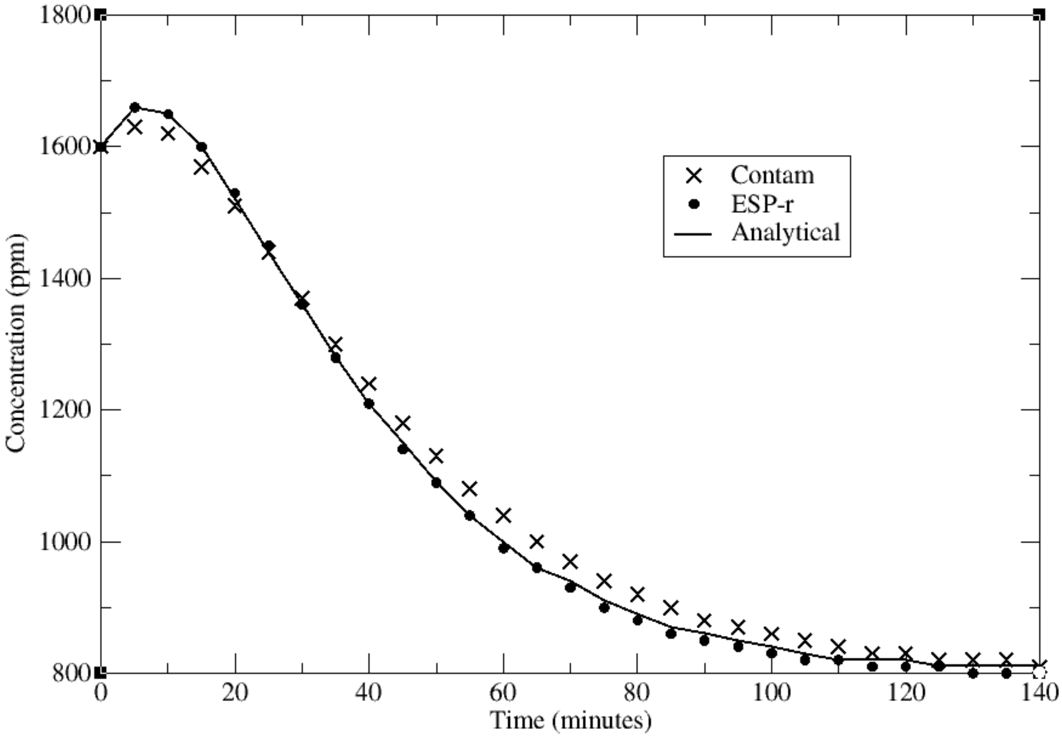


Figure 4 Results for node 5, contaminant 2 in test 4-1

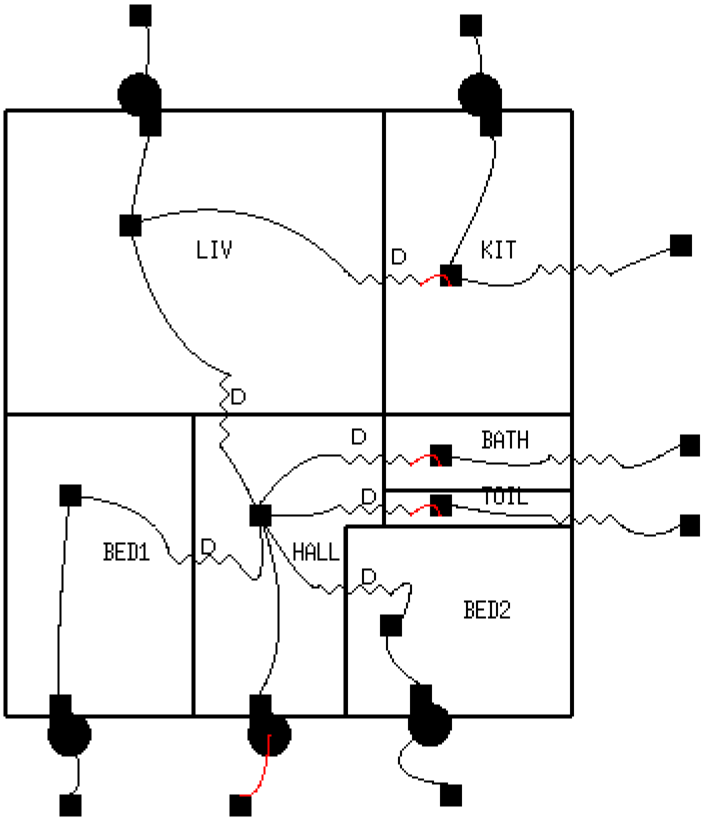
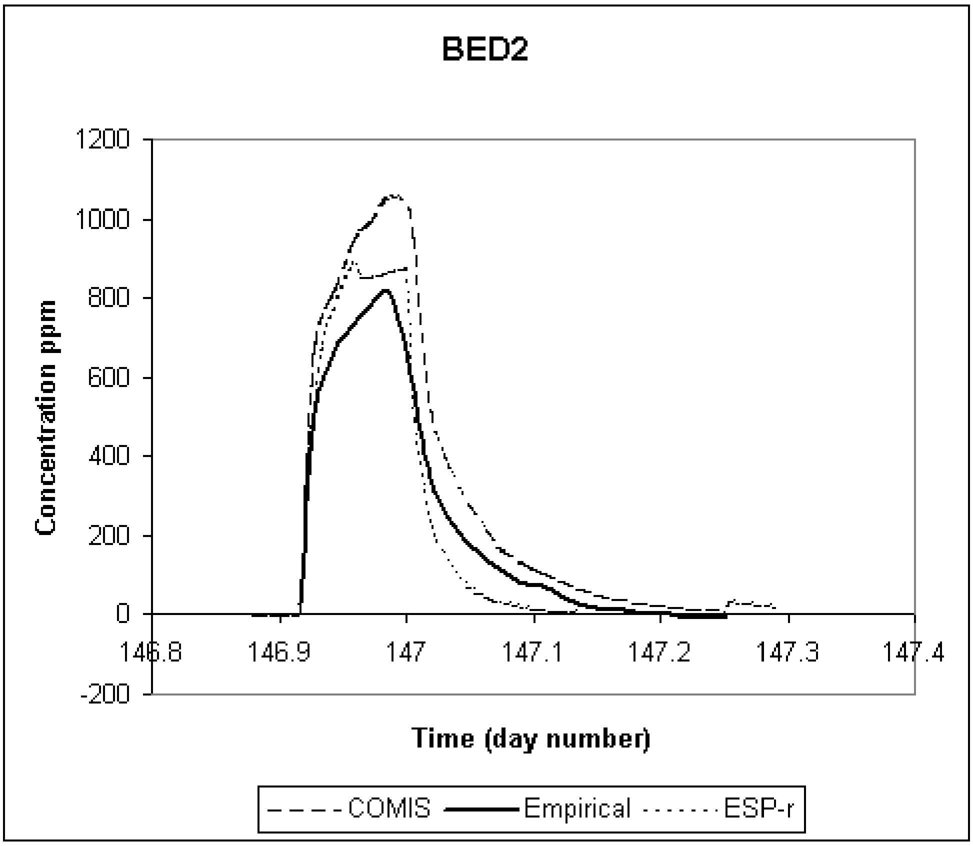


Figure 5 Plan and airflow network of experimental study

(flat in Namur, Belgium)



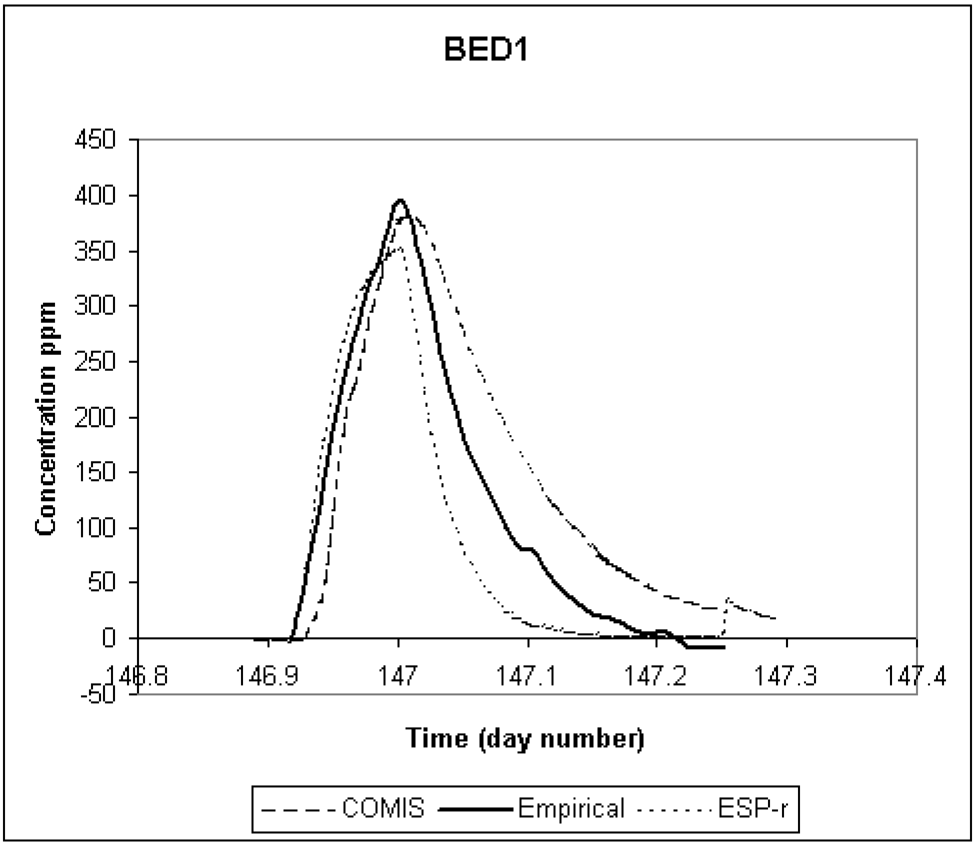


Figure 6 Transient contaminant concentrations for two zones for Namur flat

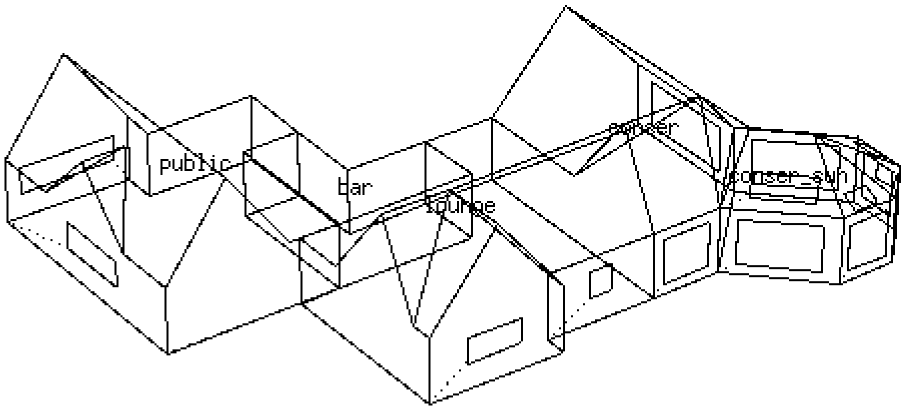


Figure 7 George and Dragon Holmes Chapel (public house in England)

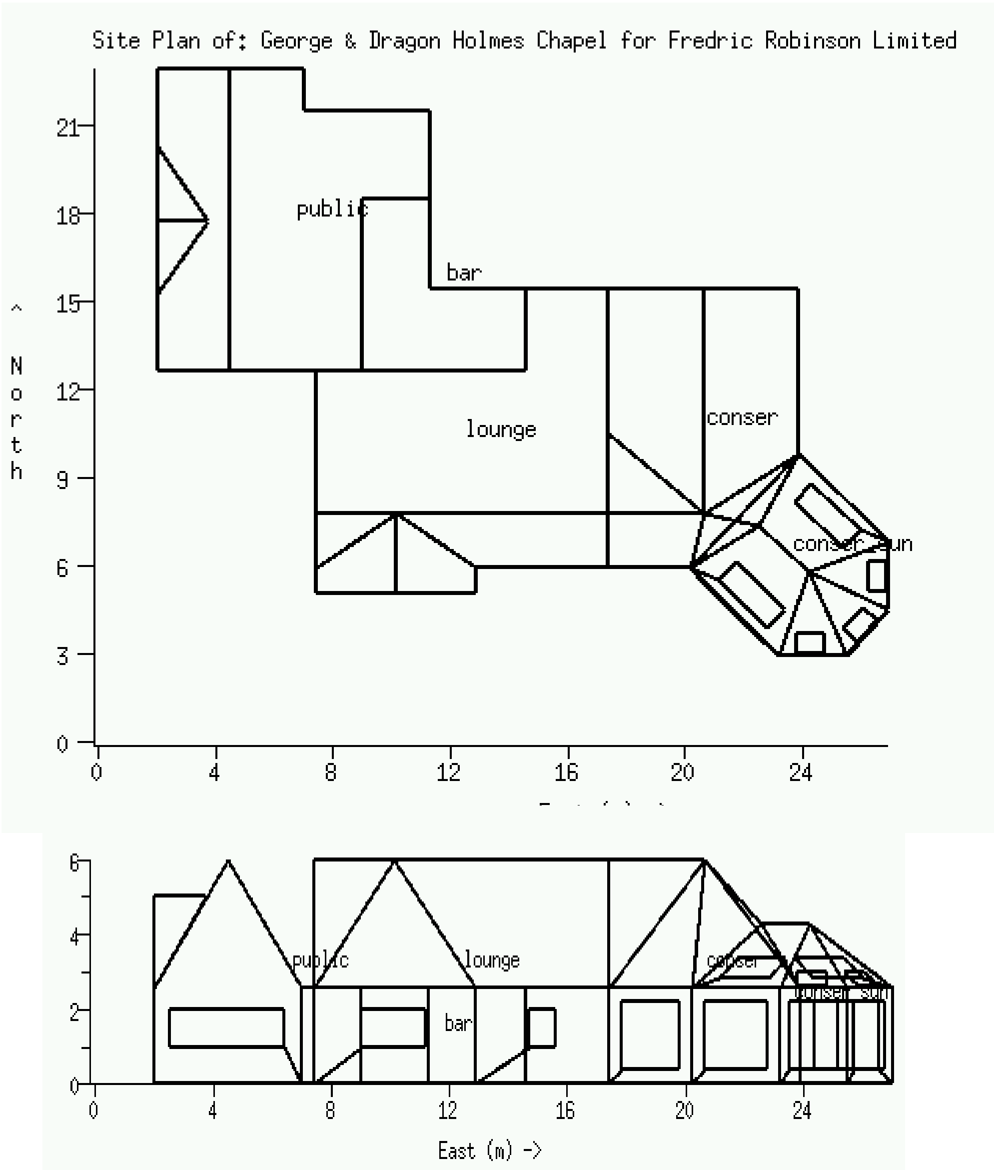


Figure 8 Plan and South elevation of public house

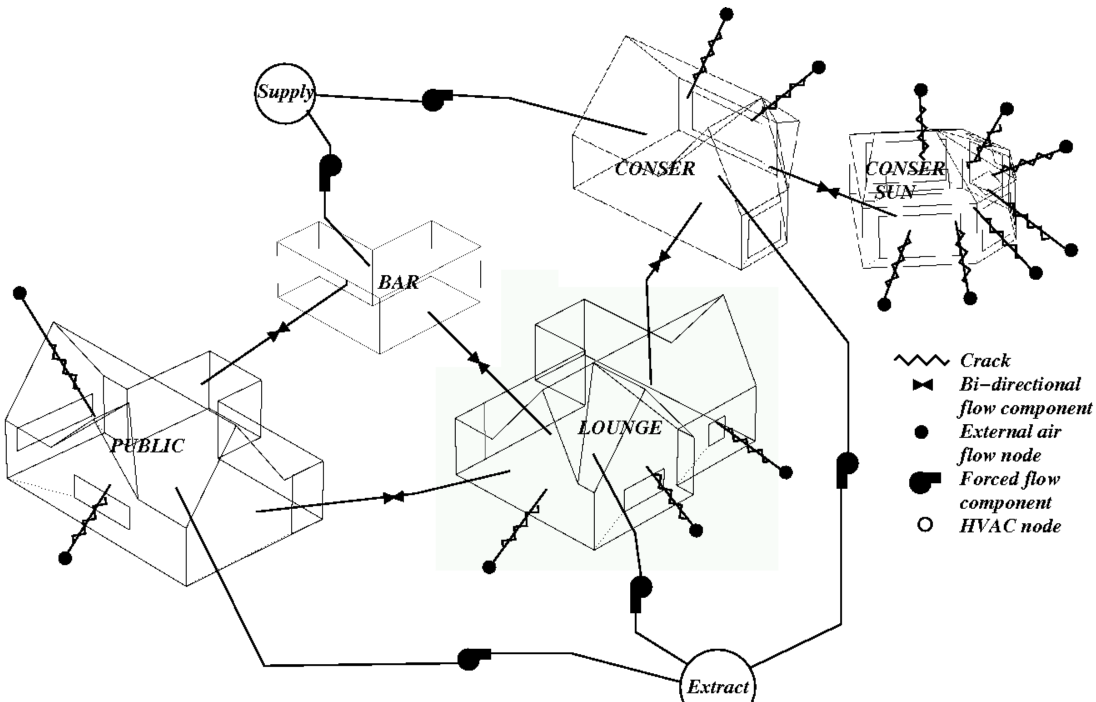


Figure 9 Air flow network for public house

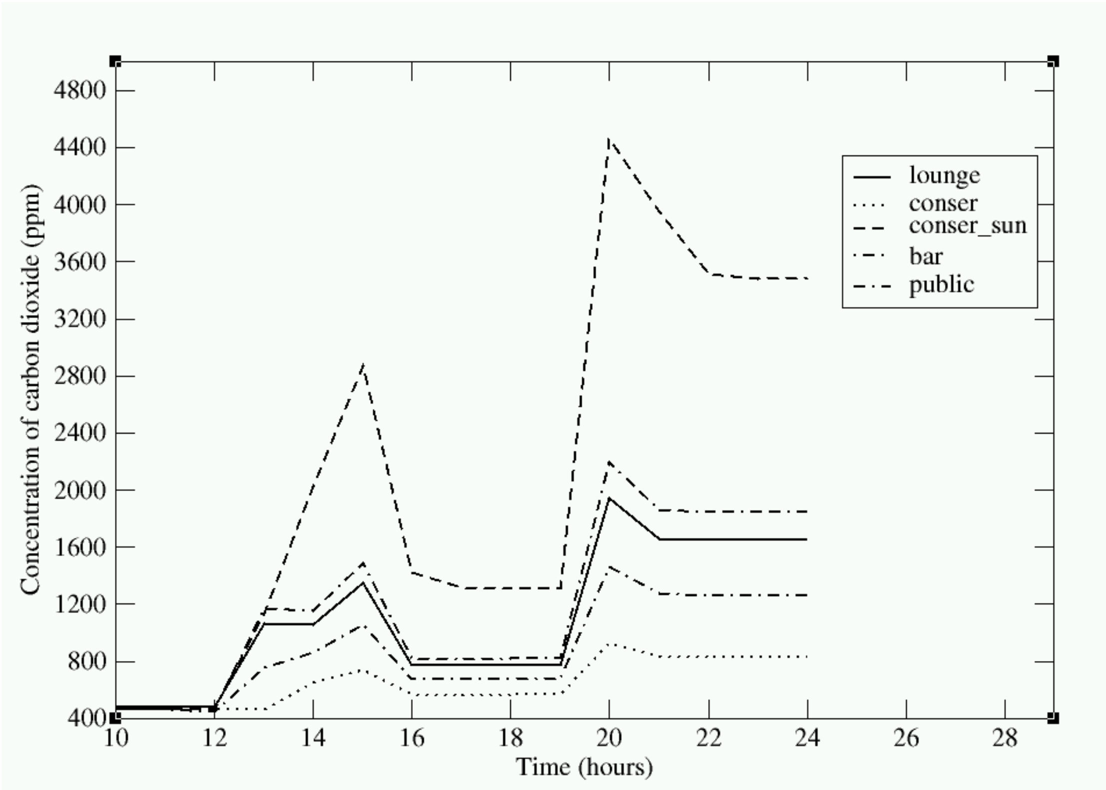


Figure 10 Concentration with temperature control

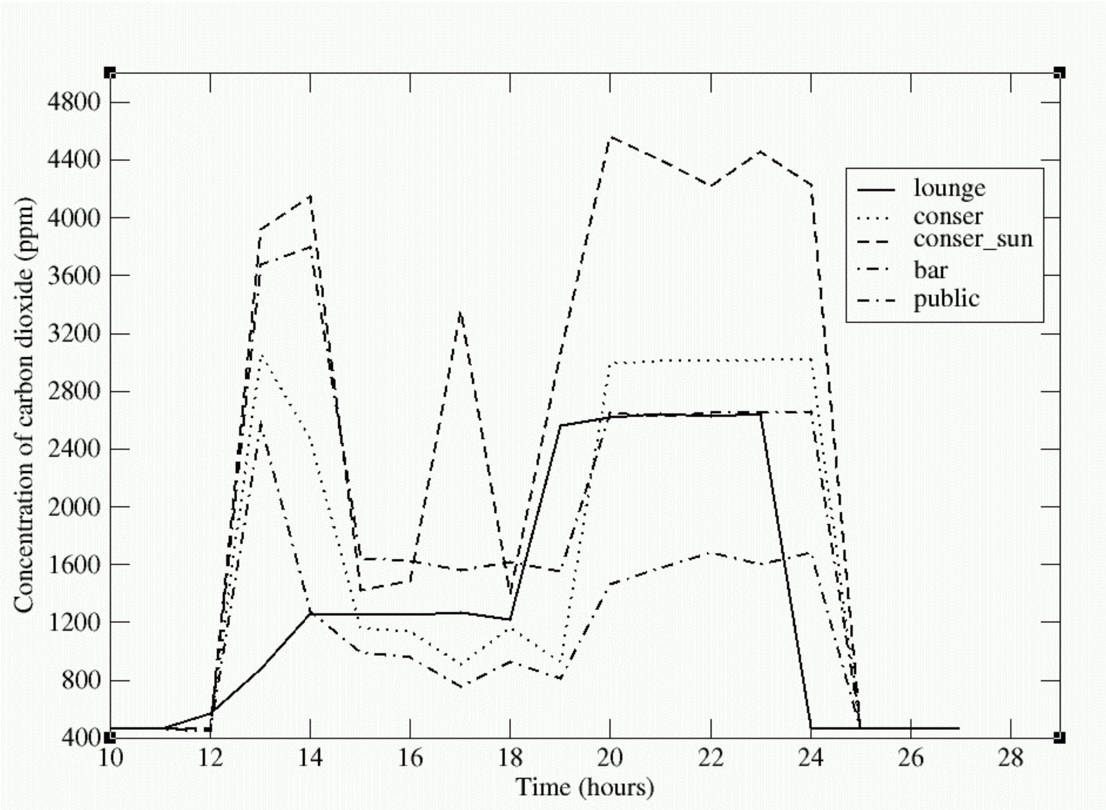


Figure 11 Concentration with occupancy based control

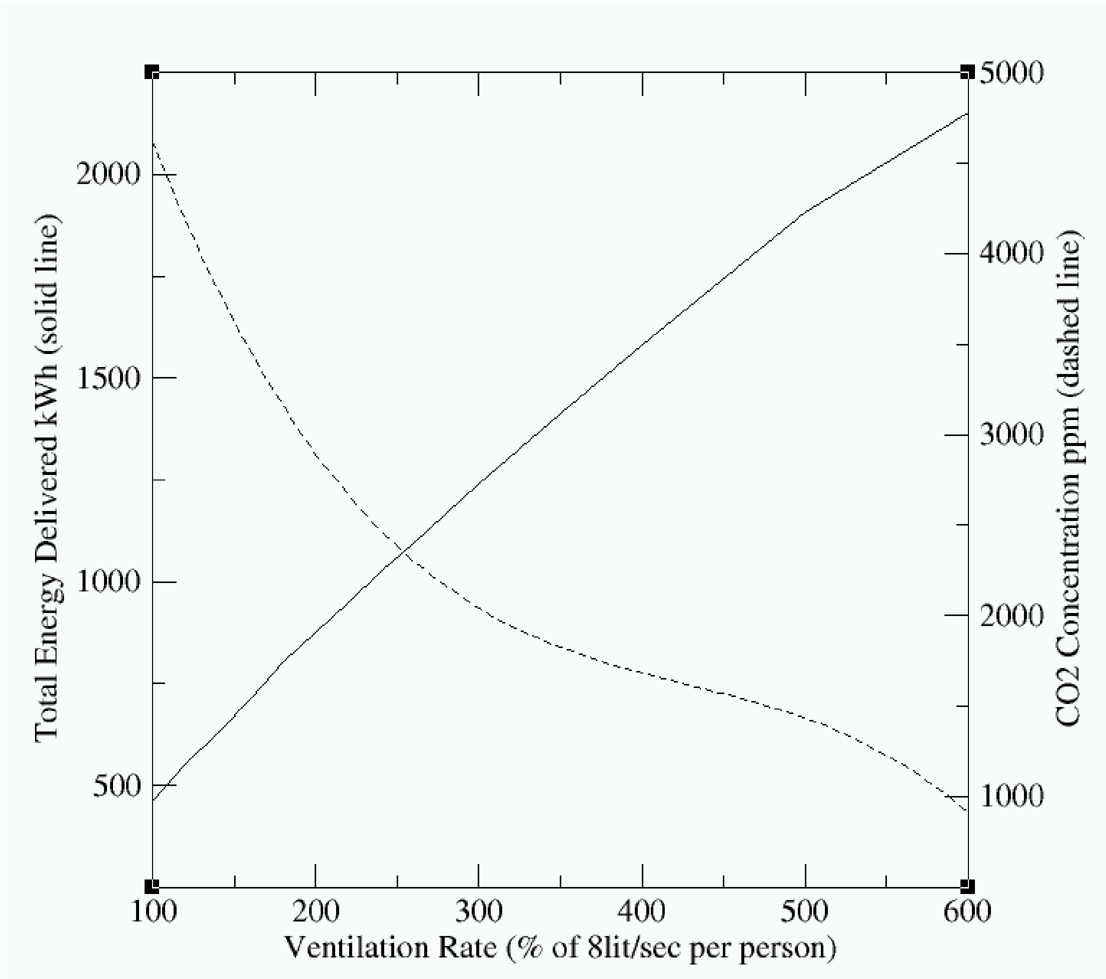


Figure 12 Heating energy vs ventilation rate

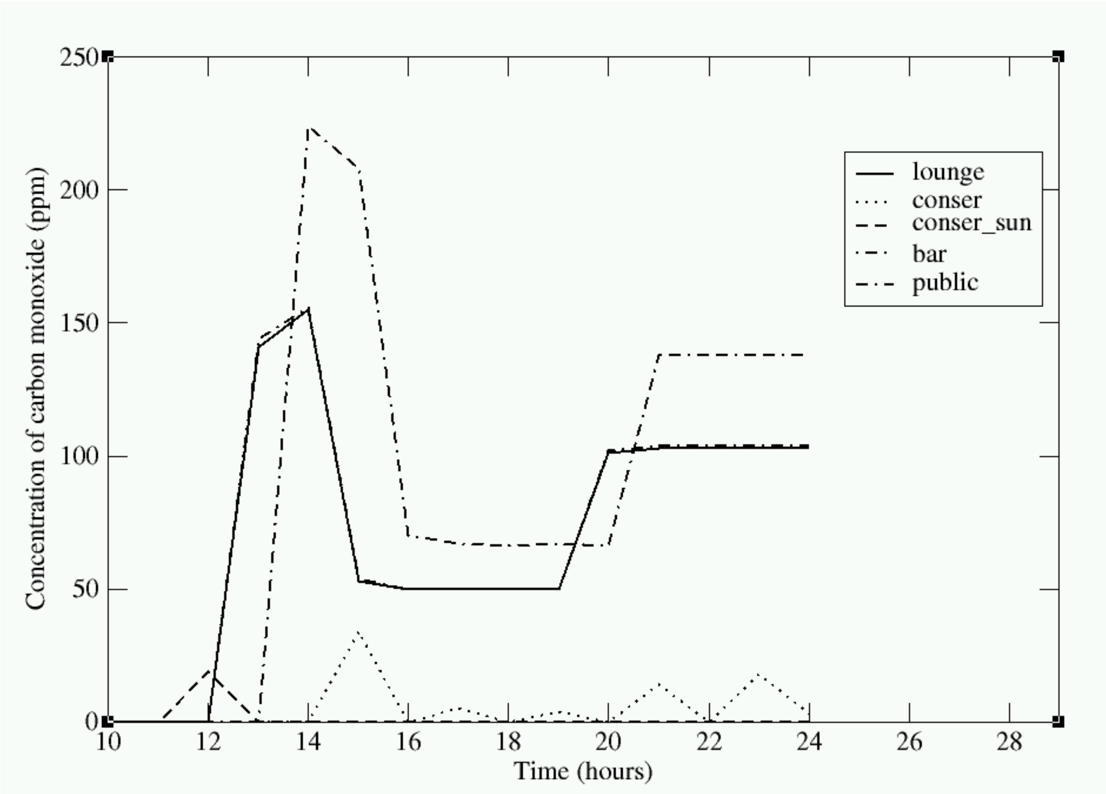


Figure 13 Carbon monoxide concentration