INTEGRATION OF CONTAMINANT BEHAVIOUR PREDICTION WITHIN WHOLE BUILDING SIMULATION

Aizaz Aamir Samuel, Paul Strachan
Energy Systems Research Unit
University of Strathclyde,
75 Montrose Street,
Glasgow, UK, G1 1XJ

ABSTRACT

Stand-alone software for predicting contaminant transport and behaviour is well developed, but to be more effective, it needs to be integrated within whole building simulation. This paper describes implementation of such a model within whole building dynamic simulation. The model is further enhanced by allowing specification of filter efficiencies, source/sink models, first order chemical reactions, contaminant based control and scheduled ambient concentration profiling. The model was validated against analytical solutions and for complex cases against CONTAM and COMIS. Empirical validation was carried out using information from IEA Task 23. The paper concludes with a case study illustrating the impact of including dynamic thermal and wind pressure conditions on predicted contaminant concentrations and flows.

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 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 sunlight on ozone (from photocopiers and printers) and on VOC (from outgassing from 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.

To study this it is important that contaminant prediction be integrated within whole building simulation and appraised along with other 'conventional' metrics.

INTEGRATED SIMULATION

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.

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.

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 as scalars. 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, results will take in account these interactions and hence be more representative of reality.

The contaminant transport model assumes that ambient contaminant concentration is a given function of time 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. A fully implicit and a fully explicit solution are also possible.

Theoretical Model

The 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 et al 2002, Walton et al 2003) model, but conflation within the whole building simulation environment ESP-r enhances contaminant modelling to include effects from aforementioned building thermodynamic domains.

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:

$$K_{ij} = -\sum m_n \qquad [i=j] \quad [N(n-1)+1 \leqslant i \leqslant Nn]$$

$$K_{ij} = k_{\alpha\beta} \qquad [i \neq j] \quad [N(n-1)<j \leqslant Nn] \quad [N(n-1)<i \leqslant Nn]$$

$$K_{ij} = m_{ln} \qquad [i \neq j] \quad [j=N(l-1)+\tilde{N}]$$

$$K_{ij} = 0 \qquad [i \neq j] \quad [j \neq N(l-1)+\tilde{N}]$$

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 (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 defined 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:

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

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 whose components on the diagonal and above remain nontrivial. The solution vector X* is then generated through backsubstitution of the known right hand side vector.

Major Limitations

Because the model bases itself on the network massflow solution algorithm, assumptions that are valid for the massflow model apply to contaminant modelling as well. Therefore at best the contaminant model can be as accurate as the underlying massflow network model. Some of the principal assumptions and limitations in this model are:

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

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

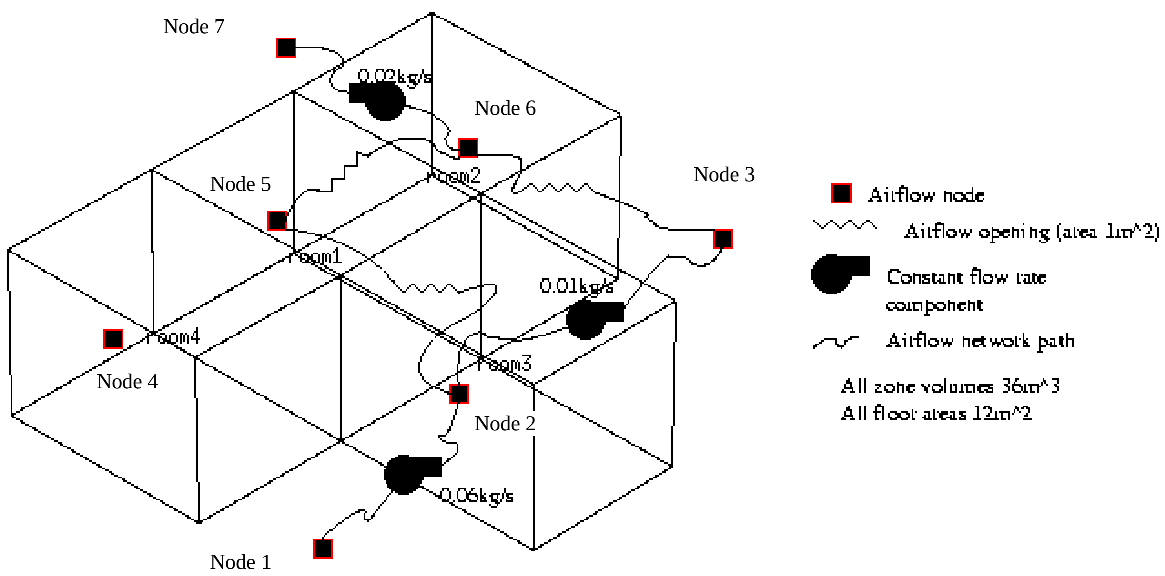

Figure 1 Project model and test cell for analytical and inter-model test

with time was compared against analytical calculations. Less than 0.1% error 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^{0}C and 1.01325bar 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:

$$C_{\alpha_2} = C_{\alpha_{amb}}(1 - e^{-k_2 t}) \quad (7)$$

$$C_{\alpha_5} = C_{\alpha_{amb}}(1 - e^{-k_5 t}(1 + k_5 t)) \quad (8)$$

$$C_{\alpha_6} = C_{\alpha_{amb}}(1 - e^{-k_6 t}(1 + k_6 t + \frac{k_6^2 t^2}{2})) \quad (9)$$

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).

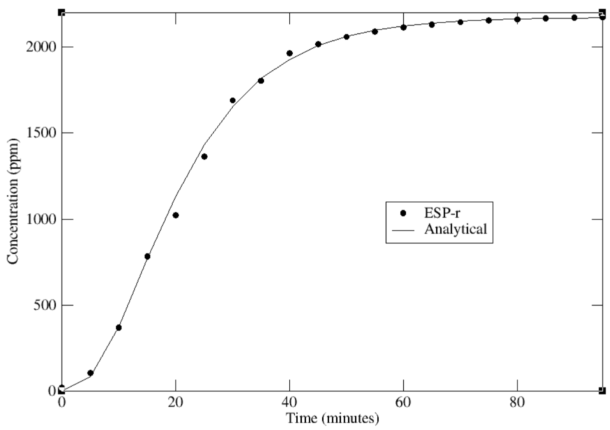

Figure 2 ESP-r & analytical results for node 2 in test 2

Convergence Checking

Convergence criteria are defined in (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^{0}C 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.

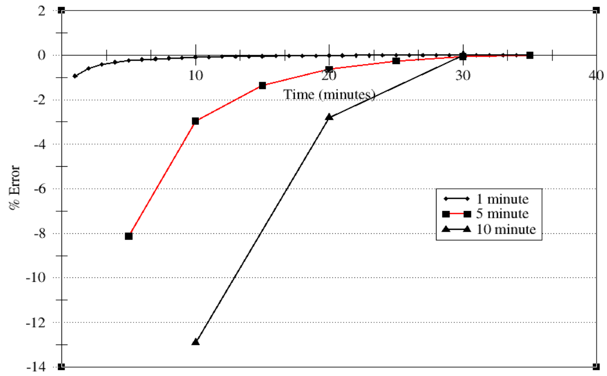

Figure 3 Effect on accuracy of reducing time step

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 in zone room1 and a source of 0.005kg/s in room2 with a cutoff concentration of 0.2kg/kg. 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 this series of tests are shown in figure 4. 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, ESP-r and the analytical solution are within a very small tolerance and fulfil the various criteria of ASTM D5157. 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.

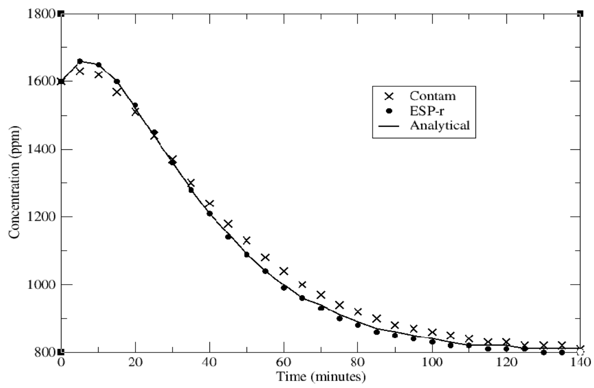

Figure 4 Results for node 5, contaminant2 in test 4-1

Empirical Validation

Results of a previously conducted study (Bossaer et al 1999) were obtained. This comprised an evaluation of a COMIS 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 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 by 2m 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.

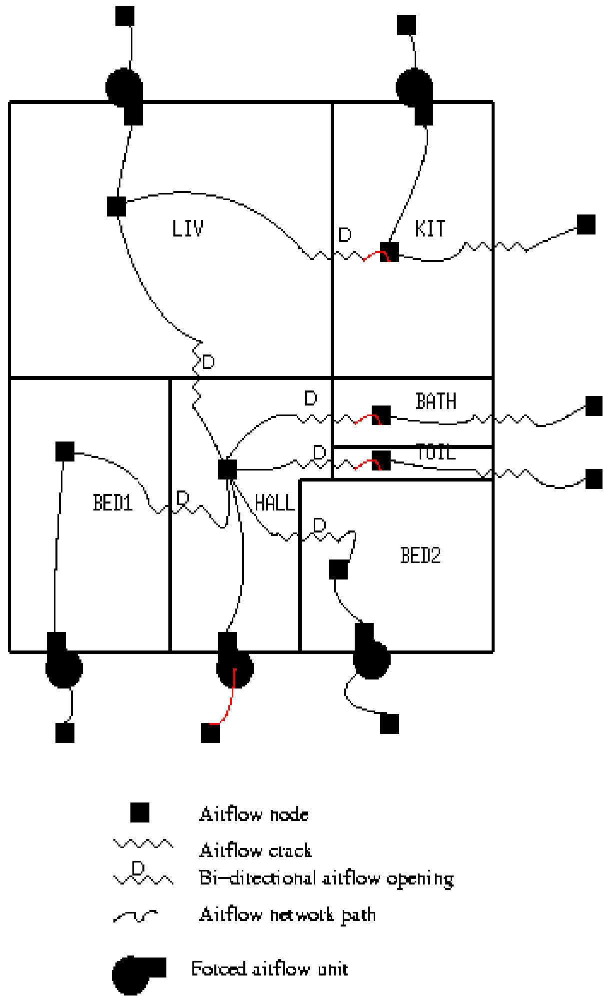

Figure 5 Plan and airflow network of experimental study (flat in Namur, Belgium)

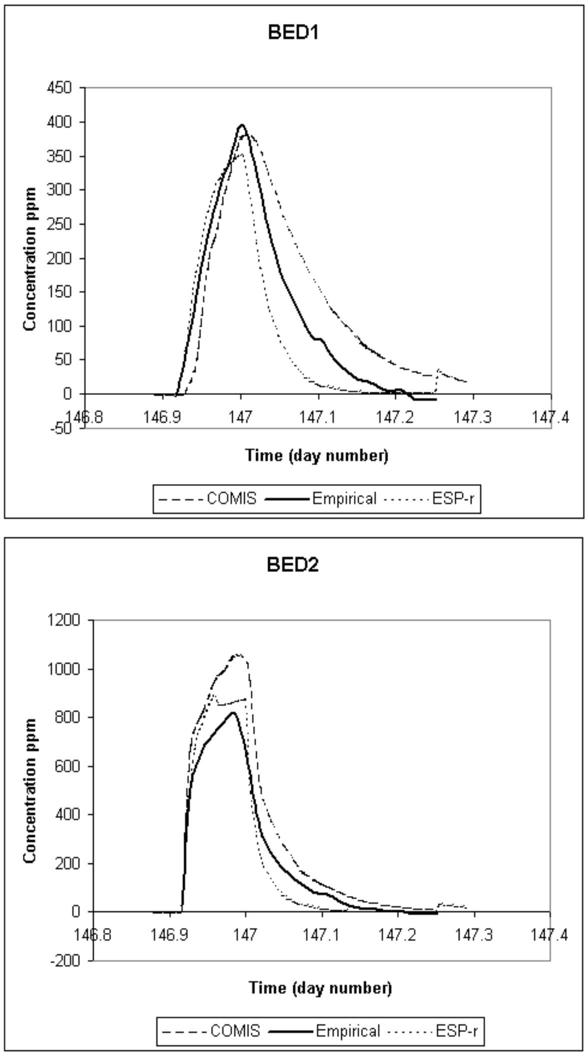

Figure 6 Transient contaminant concentrations for two zones for the Namur flat

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^{0}C. It was confirmed in the present work that temperature differences did indeed contribute remarkably to the airflow, and results quite different from the experimental were obtained until the measured temperatures were incorporated into the model. Ambient temperature was taken to be the average of the temperatures of KIT, TOIL and BATH because temperature in the other zones do not affect the airflow which is regulated by known forced flow components.

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	-96.00	-53.00	±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
	BED2		
r	0.99	0.99	0.9 or more
a	29.00	-120.00	±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

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

This tends to suggest that the measured and predicted concentrations differ significantly but correlation between these 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. It is 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

A public house in England was studied to show how CO_2 varied within occupied hours. 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. Occupants were assumed to be the only sources of $CO_{2.}$ 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 of CO_2 (Liddament 2004). The building was simulated for two days 8th and 9th of January (occupancy was considered only for one day). Ambient concentration of CO_2 was assumed to be constant at 4.6×10^{-6} kg/kg.

Figure 7 shows model detail. The building was divided into five thermal zones: public, bar, lounge, conser and conser_sun. A detailed massflow model comprising six internal and twelve external nodes was made to describe various forced and unforced air flows. A balanced HVAC system was used to define intentional air flows for the building. Thermal control was imposed on the building to maintain comfortable temperatures.It was observed that with the levels of ventilation provided (slightly less than 8l/s per person) the CO_2 levels for some parts of the occupied period rose to around ten times ambient concentration for some areas of the building.

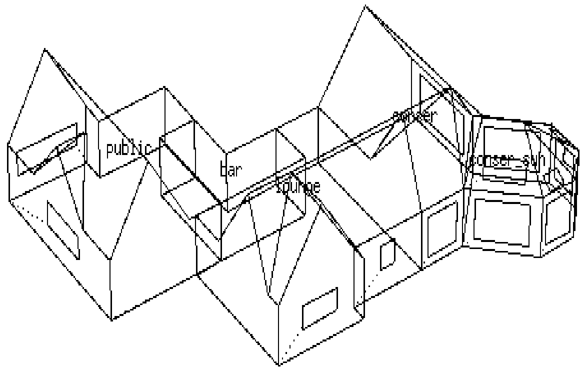

Figure 7 George and Dragon Holmes Chapel (public house in England)

The ventilation system was designed to maintain a lower pressure in the smoking parts of the building; this in turn caused CO_2 to accumulate there. The study showed that it is possible that even with typical rates of ventilation and ventilation regime, the level of CO_2 (or maybe another contaminant) may rise to significant levels. The study sheds some light on the importance of contaminant modelling. Figure 8 shows results for CO_2 concentrations.

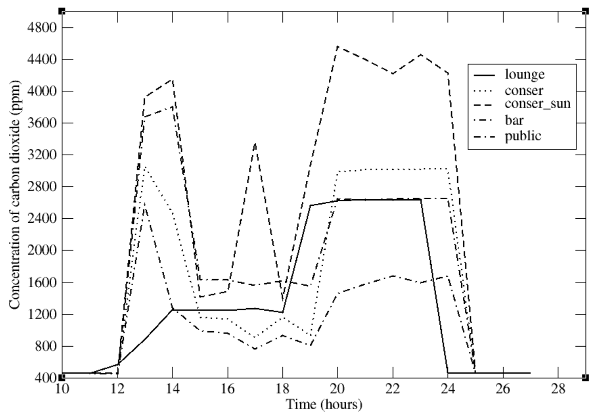

Figure 8 Temporal distribution of CO_2 in public house

CONCLUSIONS

An approach to contaminant modelling that is integrated with the 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.

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).

NOMENCLATURE

(Italics refer to symbols used in analytical solutions)

C_{α_n}	Concentration of contaminant α at node n (kg/kg)
$C_{\alpha_{amb}}$	Ambient concentration of contaminant α 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)
$k_{\alpha\beta}$	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)

REFERENCES

ASTM. 2003. D5157-97 Standard Guide for Statistical Evaluation of Indoor Air Quality Models.

Bossaer, A., Ducarme, D., Wouters, P., Vandaele, L. 1999. An Example of Model Evaluation by Experimental Comparison: Pollutant Spread in an Apartment. Energy and Buildings 30 (1999) 53-59.

Clarke, J. A. 2001. Energy Simulation in Building Design (2nd Edition). London: Butterworth-Heinneman.

Dols, W. S., Walton, G. N. 2002. CONTAMW 2.0 User Manual. National Institute of Standards and Technology, Gaithersburg, U.S.A.

Emmerich S. J., Nabinger S. J. 2001. Measurements and Simulation of the IAQ Impact of Particle Air Cleaners in a Single-Zone Building. International Journal of HVAC&R Research Vol.1, No. 7, ASHRAE.

Emmerich S. J., Nabinger S. J. 2003. Validation of CONTAMW Predictions for Trace Gas in a Townhouse. 8th International Building Performance Simulation Association IBPSA Conference. Eindhoven, The Netherlands.

EPA, 1999. Smog – Who does it hurt? EPA Washington DC, USA. EPA-452/K-99-001 July 1999.

FLUENT, 2003. FLUENT User's Manual. Fluent Inc. http://www.fluent.com

Hensen, J. L. M. 1991. On the Thermal Interaction of Building Structure and Heating and Ventilating System. PhD Thesis, Eindhoven University of Technology.

Jensen, S O. 1993. The PASSYS Project: Subgroup Model Validation and Development, Brussels. Final Report, Part I and II 1986-1992. Commission of the European Communities. DGX1I, EUR 15115 EN.

Kingsley, M., Davidson, J. 2000. Gaseous Indoor Pollutants. University of Minnesota

Liddament, M. 2004. Why CO_2? Air Infiltration Review, Volume 18, No 1, December 1996, World Wide Web Edition © Oscar Faber PLC on behalf of the International Energy Agency, 1996. http://www.aivc.org/air/18_1/mwlco2.html

McGinlay, J. 1997. The Chemistry of Atmospheric Pollutants. National Environmental Technology Centre. AEA Technologies PLC UK. http://www.aeat.co.uk/netcen/airqual/kinetics

Rogers, G. F. C., Mayhew, Y. R. 1995. Thermodynamic and Transport Properties of Fluids (SI Units) Fifth Edition. Basil Blackwell Ltd.

Versteeg, H. K., Malalasekera, W. 1995. An Introduction to Computational Fluid Dynamics. The Finite Volume Method. Prentice Hall.

Walton, G. N. 1988. Airflow Network Models for Element-Based Building Airflow Modeling. Technical Report, National Institute of Standards and Technology, Gaithersburg, U.S.A.

Walton, G. N., Dols, W. S. 2003. CONTAM2.1 Supplemental User Guide and Program Documentation. National Institute of Standards and Technology, Gaithersburg, U.S.A.

Weber, A., Koschenz1, M., Dorer, V., Hiller, M., Holst, S. 2003. TRNFLOW, A new tool for the modelling of heat, air and pollutant transport in buildings within TRNSYS. 8th International Building Performance Simulation Association IBPSA Conference, Eindhoven, The Netherlands.

Weschler, C. J., 2004. Chemical Reactions Among Indoor Pollutants: What We've Learned in the New Millennium. Indoor Air 2004; 14 (Supplementary 7); pp 184-194.