CONTAM94
A Multizone Airflow and Contaminant Dispersal Model with a Graphic User Interface

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ABSTRACT
CONTAM94 is an easily used, public domain airflow and contaminant migration analysis program. combining algorithms for modeling airflow and contaminant dispersal in multizone buildings. It employs a simplified graphic description of the building for both data entry and the presentation of simulation results. It runs on commonly available 4861 X class PC compatible computers with VGA graphics and MS-DOS. It can handle buildings containing a large number of zones.

INTRODUCTION

Over the past several years, NIST (the National Institute of Standards and Technology - formerly NBS, the National Bureau of Standards) has developed a series of public domain computer programs for calculating airflow and contaminant dispersal in multi-zone buildings. The earliest such program was ASCOS (Analysis of Smoke Control Systems) (Klote, 81). Another program, TARP (Thermal Analysis Research Program) (Walton 83), used multizone airflow calculations to estimate the portion of building thermal load due to infiltration and perform a simple contaminant migration analysis. Programs developed specifically for the study of contaminant dispersal include CONTAM86 and CONTAM87 (Axley 87 & 88). NBSAVIS/CONTAM88 (Grot, 91) added multi-zone airflow analysis capability based on TARP and a menu-driven interface to CONTAM87. Improvements in the airflow calculation algorithm were implemented in the AIRNET (Walton, 89) program. CONTAM93 (Walton, 94) combined a new graphic interface with the contaminant simulation capabilities of CONTAM88 and the airflow analysis method of AIRNET. The application of this program to a residential IAQ modeling study was discussed at the 15th AIVC Conference (Emmerich, 94). In CONTAM94 the user interface was extensively improved, and the separate interface and computation programs of CONTAM93 were combined into a single executable program.

Three basic problems have held back the use of multi-zone airflow simulations. First is the reliability and calculational efficiency of the numerical solution itself. Second is the difficulty of describing the geometric relationships of zones and airflow paths in a building in a traditional ASCII file. Third is the limited availability and questionable accuracy of data describing building airflow paths. AIRNET demonstrated a solution to the first problem; CONTAM94 demonstrates a solution to the second.

OBJECTIVE OF THE SOFTWARE

The purpose of CONTAM94 is to provide an easily used contaminant analysis program combining the best available algorithms for modeling the airflow and contaminant dispersal in multizone buildings.

TECHNICAL BASIS

The fundamental assumption in CONTAM is that the building can be modeled by some number of zones of well-mixed air. Therefore, the program stands as a compromise of accuracy, complexity, and speed between a single-zone model and a CFD (computation fluid dynamics) model of the entire building.

Mathematical Theory - Airflow Analysis

Over the years many methods have been developed to compute the building airflows which are necessary for the contaminant analysis. Feustel and Dieris (1992) report 50 different computer programs for multizone airflow analysis. Note than "zones" go by many other names in these programs, e.g., nodes, cells, and rooms are common alternatives.

The air flow rate from zone j to zone i, $w_{j,i}$ [kg/s], is some function of the pressure drop along the flow path, $P_j - P_i$:

$$w_{j,i} = f(P_j - P_i) \qquad (1)$$

The mass of air, m_i [kg], in zone i is given by

$$m_i = \rho_i V_i = \frac{P_i V_i}{R T_i} \qquad (2)$$

where

V_i = zone volume [m^3],
P_i = zone pressure [Pa],
T_i = zone temperature [K], and
R = 287.055 [J/kgK] (gas constant for air).

For a transient solution the principle of conservation of mass states that:

$$\frac{\partial m_i}{\partial t} = \rho_i \frac{\partial V_i}{\partial t} + V_i \frac{\partial \rho_i}{\partial t} \quad (3)$$

$$\sum_j w_{j,i} + F_i$$

where

m_i = mass of air in zone i,

$w_{j,i}$ = airflow rate [kg/s] between zones j and zone i: positive values indicate flows from j to i and negative values indicate flows from i to j, and

F_i = non-flow processes that could add or remove significant quantities of air from the zone.

Such non-flow processes are not considered in CONTAM94 and flows are evaluated by assuming quasi-steady conditions leading to:

$$\sum_j w_{j,i} = 0 \quad (4)$$

The steady-state airflow analysis for multiple zones requires the simultaneous solution of equation (4) for all zones. Since the function in equation (1) may be, and usually is, nonlinear, a method is needed for the solution of simultaneous nonlinear algebraic equations. The Newton-Raphson (N-R) method (Conte & de Boor, 1972, p 86) solves the nonlinear problem by an iteration of the solutions of linear equations. In the N-R method a new estimate of the vector of all zone pressures, $\{\mathbf{P}\}^*$, is computed from the current estimate of pressures, $\{\mathbf{P}\}$, by

$$\{P\}^* = \{P\} - \{C\} \quad (5)$$

where the correction vector, $\{\mathbf{C}\}$, is computed by the matrix relationship

$$[J]\{C\} = \{B\} \quad (6)$$

where $\{\mathbf{B}\}$ is a column vector with each element given by

$$B_i = \sum_j w_{j,i} \quad (7)$$

and [J] is the square (i.e. N by N for a network of N zones) Jacobian matrix whose elements are given by

$$J_{i,j} = \sum \frac{\partial w_{j,i}}{\partial P_i} \quad (8)$$

In equations (7) and (8) $w_{j,i}$ and $\partial w_{j,i}/\partial P_m$ are evaluated using the current estimate of pressure $\{\mathbf{P}\}$. The CONTAM program contains subroutines for each airflow element which compute mass flow rates and the partial derivative values for a given pressure difference input.

Equation (6) represents a set of linear equations which must be set up and solved for each iteration until a convergent solution of the set of zone pressures is achieved. In its full form [J] requires computer memory for N^2 values, and a standard Gauss elimination solution has execution time proportional to N^3. Sparse matrix methods can be used to reduce both the storage and execution time requirements. A skyline solution process following the method of Dhatt (1984, pp. 282-192) was chosen. This method can be used to solve equations with symmetric or nonsymmetric matrices. It stores no zero values above the highest nonzero element in the columns above the diagonal and no zero values to the left of the first nonzero value in each row below the diagonal. In this case the Jacobian matrix is symmetric.

Analysis of the element models will show that

$$|J_{i,i}| = \sum_{i \neq i} |J_{i,j}| \quad (9)$$

This condition allows a solution without pivoting, although scaling may be useful. Note that the degree of sparsity of the Jacobian matrix after factoring is dependent on the ordering of the zones. Ordering can be improved by various algorithms or rules-of-thumb. In AIRNET it was easy to define an airflow network which has no unique solution. The CONTAM94 graphic input makes it difficult to incorrectly connect the airflow elements in the network.

CONTAM allows zones with either known or unknown pressures. The constant pressure zones are included in the system of equations and equation (6) is processed so as to not change those zone pressures. This gives flexibility in defining the airflow network while maintaining the symmetric set of equations. A sufficient condition for the Jacobian to be nonsingular (Axley, 1987) is that all of the unknown pressure zones be linked by pressure dependent flow paths to (a) constant pressure zone(s). In CONTAM the ambient (or outside) air is treated as a constant pressure zone. The ambient zone pressure is set to zero causing the computed zone pressures to be values relative to the true ambient pressure and helping to maintain numerical significance in calculating ΔP. The true pressure in every zone must then be adjusted by this offset when evaluating zone air density.

Conservation of mass at each zone provides the convergence criterion for the N-R iterations. That is, if $\Sigma\ w_{j,i} = 0$ for all zones for the current system pressure estimate, the solution has converged. The number of iterations can be reduced and sufficient accuracy attained by testing for relative convergence at each zone:

$$\frac{|\Sigma_j w_{j,i}|}{\Sigma_j |w_{j,i}|} < \epsilon \qquad (10)$$

with a test $(\Sigma\,|w_{j,i}| < \epsilon_1)$ to prevent division by zero. The magnitude of ϵ can be established by considering the use of the calculated airflows, such as in an energy balance. In any case, round-off errors may prevent perfect convergence ($\epsilon = 0$).

Numerical tests of the N-R method solution indicated occasional instances of very slow convergence as the iterations almost oscillate between two different sets of values. In AIRNET, this was handled by a Steffensen acceleration process. More recent tests by the author and by Wray (1993) indicate that the use of a simpler constant under-relaxation coefficient produces a faster, reliable convergence acceleration process. Equation (14) for the iteration process becomes

$$\{P\}^* = \{P\} - \omega\{C\} \qquad (11)$$

where ω is the relaxation coefficient. A relaxation coefficient of 0.75 has been found to be usable for a broad range of airflow networks. This value is not a true optimum but appears to work quite well without the computational cost of finding the theoretically optimum value.

When convergence is progressing rapidly, under-relaxation ($\omega < 1$) slows convergence compared to no relaxation. To prevent this a global convergence value is computed:

$$\gamma = \frac{\Sigma_i |\Sigma_j w_{j,i}|}{\Sigma_i \Sigma_j |w_{j,i}|} \qquad (12)$$

When $\gamma^* < \alpha\gamma$, ω is set to 1. Currently CONTAM uses $\alpha = 30\%$. This often reduces the number of iterations.

Newton's method requires an initial set of values for the zone pressures. These may be obtained by including in each airflow element model a linear approximation relating the flow to the pressure drop:

$$w_{j,i} = c_{j,i} + b_{j,i}(P_j - P_i) \qquad (13)$$

Conservation of mass at each zone leads to a set of linear equations of the form

$$[A]\{P\} = \{B\} \qquad (14)$$

Matrix [A] in equation (14) has the same sparsity pattern as [J] in equation (6) allowing use of the same sparse matrix solution process for both equations. This initialization handles stack effects very well and tends to establish the proper directions for the flows. The linear approximation is conveniently provided by the laminar regime of the element models use by CONTAM, but it also may be provided by a secant approximation to the actual nonlinear behavior. When solving a set of similar problems, as when approximating a transient solution by successive steady-state solutions, it tends to be preferable to use the previous solution for the zone pressures as the initial values for the new problem.

Mathematical Theory - Contaminant Dispersal

The CONTAM93 contaminant dispersal model is an implementation of Axley's (1987, 1988) methods. He states: "The central concern of indoor air quality analysis is the prediction of airborne contaminant dispersal in buildings. Airborne contaminants disperse throughout buildings in a complex manner that depends on the nature of air movements in-to, out-of, and within the building system; the influence of the heating, ventilating, and air-conditioning (HVAC) systems; the possibility of removal, by filtration, or contribution, by generation, of contaminants; and the possibility of chemical reaction, radio-chemical decay, settling, or sorption of contaminants. In indoor air quality analysis we seek to comprehensively model all of these phenomena."

A zone is a region of uniform air temperature and contaminant concentration which may correspond to a single room, a portion of a room, or several well-coupled rooms. Selection of the zones is a matter of engineering judgement. The mass of contaminant α in zone i is

$$m_{\alpha,i} = m_i C_{\alpha,i} \qquad (15)$$

where m_i is the mass of air in zone i and $C_{\alpha,i}$ is the concentration mass fraction of α. CONTAM94 performs trace analysis only. That is, the contaminant concentration must be low enough so as not to significantly change the density of the air-contaminant mixture.

Contaminant is removed from the zone i by

(a) outward airflows at the rate $\sum_j w_{i,j} C_{\alpha,i}$ where $w_{i,j}$ rate of air flow from zone i to zone j,
(b) removal at the rate $C_{\alpha,i} R_{\alpha,i}$ where $R_{\alpha,i}$ is a removal coefficient, and
(c) first-order chemical reactions with other contaminants $C_{\beta,i}$ at the rate $m_i \sum_\beta \kappa_{\alpha,\beta} C_{\beta,i}$ where $\kappa_{\alpha,\beta}$ is the kinetic reaction coefficient in zone i between species α and β. (Sign convention: positive κ for generation and negative κ for removal)

Contaminant is added to the zone by:
(a) inward airflows at the rate $\sum_j (1-\eta_{\alpha,j,i}) w_{j,i} C_{\alpha,j}$ where $\eta_{\alpha,j,i}$ is the filter efficiency in the path from zone j to zone i,
(b) generation at the rate $G_{\alpha,i}$, and
(c) reactions of other contaminants.

Conservation of contaminant mass for each species (and assuming trace dispersal - $m_{\alpha,i} \ll m_i$) produces the following basic equation for contaminant dispersal in a building: (16)

$$\frac{dm_{\alpha,i}}{dt} = -R_{\alpha,i}C_{\alpha,i} - \sum_j w_{i,j}C_{\alpha,i} + \sum_j w_{j,i}(1-\eta_{\alpha,j,i})C_{\alpha,j} + m_i \sum_\beta \kappa_{\alpha,\beta} C_{\beta,i} + G_{\alpha,i}$$

This differential equation is approximated by an implicit difference equation. There is one such equation for every contaminant in every zone. These equations must be solved simultaneously for all zones and contaminants.

There are two major limitations in the equations presented above. First is constant zone air mass. This is consistent with the zone temperatures being constant and contaminant mass fractions being low. Second is the use of linear analysis which limits the kinds of kinetic reactions which can be modeled.

CONTAM allows the user to define the generation, G_α, and removal, R_α, coefficients for some simple cases. The general source/sink model uses the following equation:

$$S_\alpha = G_\alpha - R_\alpha \cdot C_\alpha \qquad (17)$$

where S_α is called the contaminant α "source strength". The CONTAM internal units for the terms in equation (17) are: C_α [kg_α/kg_{air}], G_α, S_α [kg_α/s], and R_α [kg_{air}/s]. The user may express these values in a large number of units with automatic conversion to the internal values. For a room air filtering device, G = 0.0 and R = f · e where f is the flow rate of the room air passing through the filter and e is the single pass removal efficiency of the device. Some other source/sink models are available.

CONTAM94 maintains the same equation ordering for the contaminant equations as is used for airflows except that for each zone there is an equation for each contaminant species. These simultaneous equations are solved by the non-symmetric skyline method.

Graphic Interface

When using CONTAM94, the user does not directly access the ASCII data file describing the building. All access to the building description is done through the program and its graphic interface. The description of the building is created (or modified) in the SketchPad. The SketchPad consists of an invisible array of small cells into which the user places various symbols representing building features relevant to the calculation of airflow and contaminant dispersal. This produces a simple illustration which has been chosen intentionally to represent the simplicity of the underlying mathematical model. The SketchPad is used to establish the geometric relationships of the relevant building features. It is not intended to produce a scale drawing of the building. Instead, it is used to create a simplified model where the walls, zones, and airflow paths are topologically similar to the actual building. The SketchPad allows the entry and display of the data in an intuitive manner. The SketchPad brings up various data entry screens needed to define the mathematical characteristics of the various building features (e.g. leakage areas and contaminant source strengths). After performing the simulation, the flows and pressure drops at each opening are presented on the SketchPad. Transient contaminant concentrations can also be displayed as separate graphs. Context sensitive, on-screen help is always available.

The CONTAM94 SketchPad is designed to simplify the data input and analysis processes for a multi-zone airflow and contaminant dispersal simulation. It is still up to the user to decide how best to idealize the building as a multizone system based on the building layout and the objectives of the simulation. The user must also determine which contaminant dispersal processes are important and appropriate input values for the building being simulated. The required input values can be numerous and include the following: airtightness of exterior envelope and interior partition components, ventilation system airflow rates, wind pressure coefficients, ambient weather and contaminant concentrations, indoor contaminant source strengths and sink characteristics, contaminant reaction rates, and filter efficiencies. Values of these quantities can be estimated from the published literature and field measurement.

Once the user has decided how to represent the building as a multizone system and has determined appropriate input values, the building data is entered into the SketchPad. Building data is organized by levels with data entry beginning at the lowest level. A level would typically be a building floor, but a suspended ceiling acting as a return air plenum or a raised floor acting as a supply plenum may also be treated as a level leading to multiple levels per floor. Each level is divided by walls into separate regions of uniform air temperature, pressure, and contaminant concentration called zones. Walls include the building envelope and internal partitions with a significant resistance to air flow, and are drawn as either horizontal or vertical lines.

Figure 1 shows one level of a building modeled as 9 zones: 3 zones (perhaps office areas) on either side of a hallway zone, with a zone representing an elevator shaft at the left end of the hall and a stairshaft zone at the right end. Consider this to be the second- level of a building. The zones on different levels are normally separated by floors. These zones are represented by the type (a) icons. At the zone icon, the user enters data about the zone temperature, volume, and initial contaminant concentrations. Icon (b) indicates there is no floor between this level and the level below, which means that the zone is actually part of the zone below and there is no resistance to airflow between levels for this elevator shaft. A default ambient zone surrounds the building. Other zones can be designated as ambient to represent, for example, a courtyard.

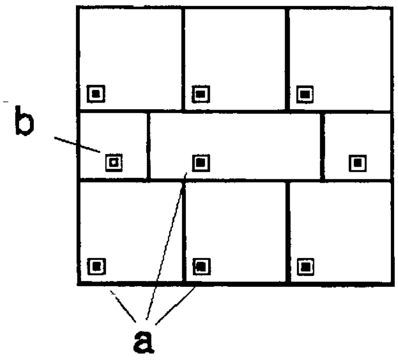

Figure 1 Walls and Zone Icons

An airflow path indicates some building feature by which air can move from one zone to another. Such features include cracks in the building envelope, open doorways, and exhaust fans. In figure 2 the type (a) icons which have been placed on the walls represent openings between zones or to ambient; icon (b) represents an opening in the floor to the zone on the level below to allow an inter-level flow. Icon (c) in the stairshaft has been set by the user to indicate a large opening betweens levels to indicate a low resistance to airflow. The type (d) icons indicate paths which can allow a two-way flow between zones with different temperatures. At the path icon the user enters data describing the flow/pressure relationship, the height of the path relative to the current level, and a wind pressure data which will be used to convert wind speed and angle to pressure on envelope openings.

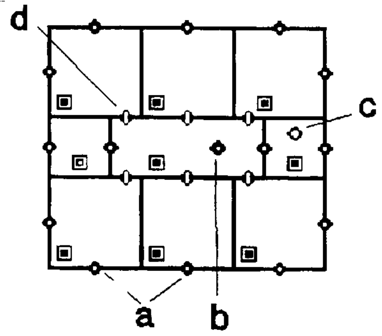

Figure 2. Airflow Paths

A simple model of an air handling system is available with supply and return point symbols placed within the appropriate zones. Icon (a) in figure 3 represents the implicit supply and return zones in such an air handling system, which are placed independent of the building zones. The supply zone is implicitly connected to all the icon (b) supply points, and the icon (c) return point is connected to the return zone. At the return zone some air may be exhausted and some recirculated; at the supply zone some outdoor air enters the system. All supply and return airflows follow user defined schedules.

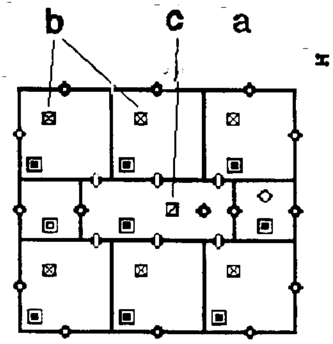

Figure 3 Simple AHS

Contaminant source (or sink) icons, (a) in figure 3, may be placed in any zone. These represent any feature (within the list of available models) which produces, removes, or adsorbs a contaminant.

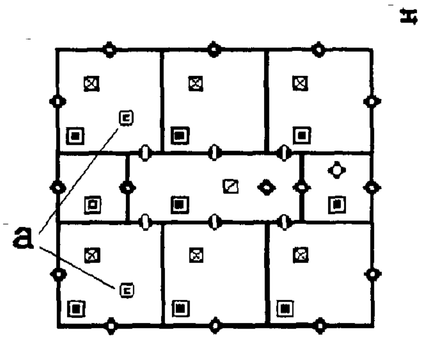

Figure 4. Contaminants

The description of large buildings is helped by the ability to copy or move individual icons and to copy entire building levels.

Although the airflow network can be considered as a traditional graph, it is believed that the graphic presentation in CONTAM94 will be more easily understood, especially for large buildings, than traditional graphic representations.

EXTENSIONS

Work is presently underway to improve the usability and the completeness of the program. CONTAM95 will include libraries of airflow paths and contaminant source/sink models. Extensions in the simulation capabilities will include detailed ductwork models, and exposure and non-trace contaminant analysis. Theoretical approaches for non-linear contaminant chemistry and aerosol transport have been developed. Inclusion of a simple thermal analysis would also be desirable.

AVAILABILITY

CONTAM94 requires a 386 class (or higher) PC compatible computer with math coprocessor (preferably 486DX), VGA graphics, and MS-DOS. It uses a DOS extender to allow the development of simulations limited only by the size of available memory. However, it cannot be run from Windows because of a conflict with the Windows memory manager.

CONTAM94 is most quickly available via FTP on the Internet. Contact gwalton@enh.nist.gov for instructions. Otherwise, call George Walton at 301-975-6421 for a disk.

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REFERENCES

Axley, J., "Indoor Air Quality Modeling, Phase II Report", US National Bureau of Standards Report NBSIR 87-3661, 1987.

Axley, J., "Indoor Air Quality Modeling, Phase III Report", US National Bureau of Standards Report NBSIR 88-3814, 1988.

Conte, S.D. and C. de Boor. 1972. *Elementary Numerical Analysis*, McGraw-Hill, New York NY, pp 299-306.

Dhatt, G., G. Touzot, & G. Catin. 1984. *The Finite Element Method Displayed*, John Wiley & Sons, New York.

Emmerich, S.J., A.K. Persily, G.N. Walton, "Application of a Multi-zone Airflow and Contaminant Dispersal Model to Indoor Air Quality in Residential Buildings", *15th AIVC Conference - The Role of Ventilation*, Buxton, UK, 27-30 Sept, Vol 2, 1994.

Feustel, H.E. & J. Dieris. 1992. "A survey of airflow models for multizone structures", *Energy and Buildings*, Vol 18, pp 79-100.

Grot, R.A., "User Manual NBSAVIS CONTAM88", National Institute of Standards and Technology, NISTIR 4585, 1991.

Klote, J.H., "A Computer Program for Analysis of Smoke Control Systems", NBSIR 80-2157, National Bureau of Standards (U.S.), 1981.

Walton, G.N., "Thermal Analysis Research Program Reference Manual," NBSIR 83-2655, National Bureau of Standards, 1983.

Walton, G.N., "AIRNET - A Computer Program for Building Airflow Network Modeling", National Institute of Standards and Technology, NISTIR 89-4072, 1989.

Walton, G.N., "Airflow Network Models for Element-Based Building Airflow Modeling", *ASHRAE Transactions*, Vol. 95, Pt. 2, 1989.

Walton, G.N., "CONTAM93 User Manual", National Institute of Standards and Technology, NISTIR 5385, 1994.

Wray, C.P. & G.K. Yuill. 1993. "An Evaluation of Algorithms for Analyzing Smoke Control Systems", *ASHRAE Transactions*, Vol 99, Pt 1.