

A Tool for Modeling Airflow & Contaminant Transport

By **W. Stuart Dols**
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Multizone modeling refers to analysis techniques that use a simplified, zonal representation of a building to study building airflows, pressure differences, and contaminant transport. Each zone is assumed to have uniform temperature, pressure, and contaminant concentrations. Zones typically represent individual rooms but can be entire levels depending on the building layout and the goals of the modeling. Zones are connected through flow paths represented mathematically by pressure-flow relationships. This article describes CONTAMW [Dols et al. 2000], a multizone modeling tool.

It is important to distinguish multizone modeling from computational fluid dynamics (CFD) modeling [Emmerich 1997]. CFD is a microscopic modeling technique that provides a more detailed representation of the airflow, temperature, and contaminants in a zone using hundreds or thousands of nodes per zone.

CFD analysis tools solve the system of mass, energy, and momentum conservation equations known as the Navier-Stokes equations to determine the air velocity, temperature and contaminant concentration at each of these nodes.

Multizone modeling is a macroscopic technique that treats each zone as a node in a system of mass balance equations. Multizone modeling is suited to applications that require knowledge on a whole building scale.

For example, multizone modeling could be used to gain insight into the transport of contaminants throughout an entire

building. CFD modeling would be used to model the behavior of a contaminant within a single room.

What is CONTAMW?

CONTAMW is the latest version in a family of multizone indoor air quality and ventilation analysis computer programs developed by the Building and Fire Research Laboratory of the National Institute of Standards and Technology (NIST) [Axley 1988, Walton 1995 and 1997]. The program provides the ability to create multizone models of a building and simulate interzonal airflow and contaminant transport. It employs a graphical user interface that simplifies the task of developing the zonal representation of a building.

This user interface implements a SketchPad that lets the user draw schematic floor plans and establish the geometric relationships of relevant building

features such as zones, airflow paths, ventilation systems, contaminant sources, and building occupants. CONTAMW translates the SketchPad diagram into a system of equations that model the building system when performing simulations.

Basic Theory

CONTAMW performs a simultaneous mass balance of air in all zones to determine zone pressures and airflow rates through each airflow path. Airflows and contaminant information are then used to determine contaminant concentrations within the zones. The following is a brief explanation of the method. It is presented in detail in Walton (1989) and Axley (1988).

The mass flow rate from zone j to zone i , $w_{j,i}$, along a given airflow path is a function of the pressure difference between the zones ($\Delta P_{j,i} = P_j - P_i$).

$\Delta P_{j,i}$ is assumed to be governed by the Bernoulli equation, which accounts for static pressure on each side of the flow path, pressure differences due to density and height differences, and pressure differences due to wind.

Conservation of mass is applied for all zones leading to a set of nonlinear algebraic equations that must be solved iteratively. CONTAMW uses the Newton-Raphson method to solve for the zonal

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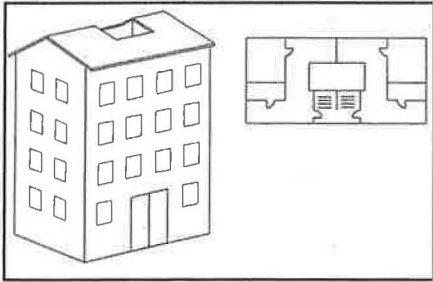


Figure 1: Sketch and floor plan of the building to be analyzed.

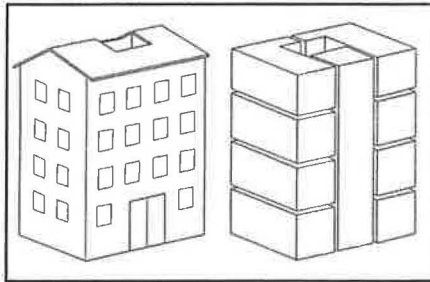


Figure 2: Less detailed building idealization.

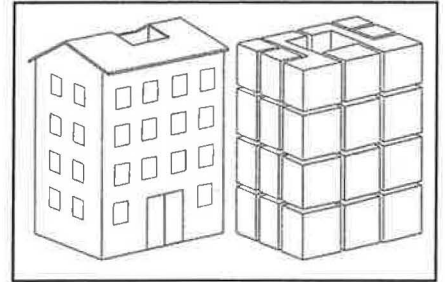


Figure 3: More detailed idealization of the building.

pressures and mass flow rates for all zones and airflow paths respectively.

Once the mass flow rates are computed, contaminant concentrations can be computed based on conservation of mass for each contaminant in each zone.

The mass of contaminant α in zone i is

$$m_{\alpha,i} = m_i \times C_{\alpha,i} \quad (1)$$

where m_i is the mass of air in zone i , and $C_{\alpha,i}$ is the concentration mass fraction of α .

Contaminant is removed from zone i by:

1. Outward airflows from the zone at a rate of $\sum_j F_{i,j} \times C_{\alpha,i}$ where $F_{i,j}$ is the rate of airflow from zone i to zone j .

2. Removal at the rate $C_{\alpha,i} \times R_{\alpha,i}$ where $R_{\alpha,i}$ is a removal coefficient.

3. First-order chemical reactions with other contaminants $C_{\beta,i}$ at the rate $m_i \times \sum_b \kappa_{\alpha,\beta} \times C_{\beta,i}$ where $\kappa_{\alpha,\beta}$ is the kinetic reaction coefficient in zone i between species α and β .

Contaminant is added to the zone by:

1. Inward airflows at the rate $\sum_j (1 - \eta_{\alpha,j,i}) F_{j,i} \times C_{\alpha,j}$ where $\eta_{\alpha,j,i}$ is the filter efficiency for contaminant α in the path from zone j to zone i .

2. Generation at the rate $G_{\alpha,i}$.

3. Reactions of other contaminants.

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

$$\frac{dm_{\alpha,i}}{dt} = -R_{\alpha,i} C_{\alpha,i} - \sum_j F_{i,j} C_{\alpha,i} + \sum_j F_{j,i} (1 - \eta_{\alpha,j,i}) C_{\alpha,j} + m_i \sum_{\beta} \kappa_{\alpha,\beta} C_{\beta,i} + G_{\alpha,i} \quad (2)$$

This differential equation is approximated by a difference equation and solved using a fully implicit numerical approximation.

Model Assumptions

CONTAMW implements mathematical relationships to model airflow and contaminant related phenomena. It incorporates the following assumptions that simplify the model:

Well-mixed zones. Each zone is treated as a single node with uniform (well-mixed) conditions throughout. These conditions include temperature, pressure, and contaminant concentrations. CONTAMW cannot account for localized effects within a zone. For example, if a mass of contaminant is introduced into a zone at a certain time (burst source), CONTAMW assumes the con-

taminant will be mixed into the entire volume of the zone within a single time-step.

Trace contaminants. Currently, CONTAMW handles only *trace contaminants* (i.e., those found at low enough concentrations that they do not affect the density of air within a zone). Care must be taken not to rely on the model to handle contaminant concentrations that would change the density of the air (e.g., moisture and thick smoke). The program treats contaminants as trace contaminants even if it calculates concentrations that would affect the density. CONTAMW calculates the contaminant concentration as the ratio of the mass of contaminant to the volume of the zone. The calculated mass of air within the zone will not change because the model maintains each zone at a constant temperature and volume. It assumes differences due to changes of pressure within a zone are negligible.

Heat transfer. The model does not handle *heat transfer* phenomena. The temperatures in all zones are constant as set by the user. Different zones can be set to different temperatures, but they remain constant throughout a simulation. The model does determine airflows induced by temperature differences between zones (including ambient) as caused by the stack effect.

Element models. Airflow path and source/sink elements are each represented by mathematical models. Users must use models appropriate for their applications.

These assumptions relate to the mathematical representations that CONTAMW uses and should be distinguished from assumptions that users make when creating a model. Users must exercise engineering judgment so the building representation is adequate for the purposes of the analysis.

Using CONTAMW

The following is a brief overview on the use of CONTAMW to develop a building representation and perform a simulation. Five distinct tasks are required to perform a multizone analysis with CONTAMW:

1. Develop a building idealization,
2. Draw schematic representation,
3. Define building components,
4. Perform simulations, and
5. Review results.

Figure 1 shows a sketch of a four-story building that will be used for this discussion.

Icon Category	Component Icons
Walls	
Zones	
Duct Segments	
Duct Junctions	
Duct Terminals	
Simple AHS	
Airflow Paths	
Source/Sinks	
Occupants	

Table 1: Building component icons used for SketchPad representations.

Task 1 – Building Idealization

Building idealization refers to representing a building as a set of zones and airflow paths that are relevant to the goal of the analysis. A building can be idealized in many ways depending on the building layout, the ventilation system configuration, and the problem of interest. For example, the simple idealization shown in Figure 2 could be used to study building envelope leakage and stack effect within the stair shaft.

Figure 3 shows a detailed idealization in which each room is a single zone. This idealization accounts for airflows between rooms. The idealization could be even more detailed to include plenums, wall cavities, and chases [Musser and Yuill 2000].

During this stage of model development, consideration is given to the connections and leakage paths between zones, including the outdoors. These leakage paths can be represented in various levels of detail that range from accounting for each building component to combining leakage elements into a single leakage value for the interface between two zones.

For example, one could represent each window, door, and wall penetration individually. Alternatively, one could determine the distributed leakage rate on a square meter basis and enter a single value for the façade on each level of the building. Sources of leakage information include building specific measurements, effective leakage area tables, literature, and engineering judgment [Persily and

Ivy 2001]. Chapter 25 of the *ASHRAE Handbook—Fundamentals* [ASHRAE 1997] provides a table of effective leakage areas of building components.

Task 2 – SketchPad Representation

After developing a building idealization, the next step is to draw a schematic representation on the SketchPad. Typi-

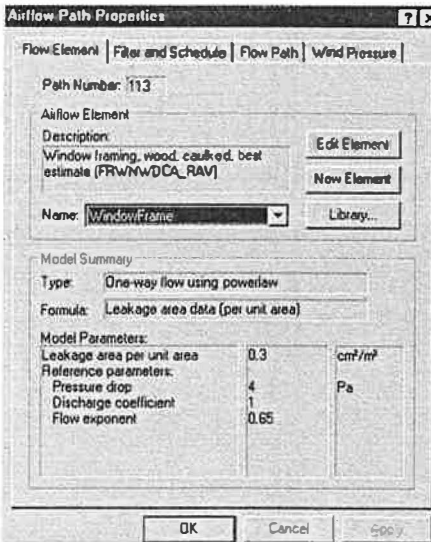


Figure 5: Airflow path property sheet.

cally a floor plan is drawn for each level of the building representing each room as a zone. Building component icons are placed on the SketchPad to represent zones, airflow paths, and mechanical ventilation system components. Table 1 shows the icons CONTAMW uses to represent building components.

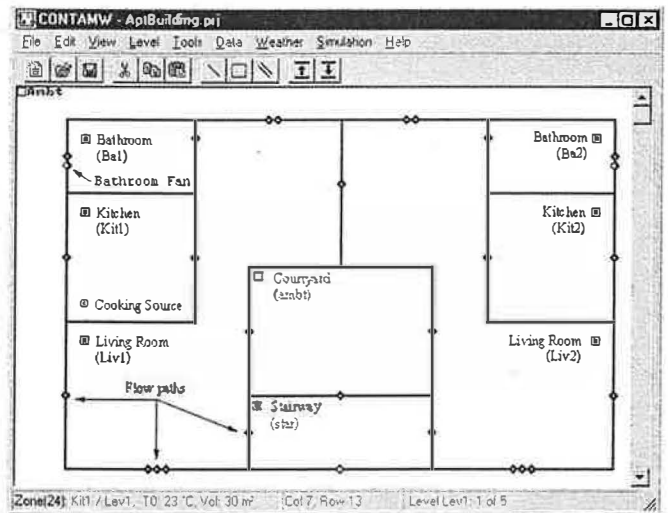


Figure 4: SketchPad representation of a typical floor.

Figure 4 shows the SketchPad representation of a floor plan based on the idealization in Figure 3. To simplify the data input process in multi-story buildings, CONTAMW provides the ability to copy levels. A user can draw a typical level, copy it, and make modifications necessary to account for differences between levels.

Task 3 – Define Components

Each icon on the SketchPad is a building component with associated parameters that define its characteristics. Parameters are entered via building component property sheets (Figure 5) that are accessed by double-clicking on an icon. To simplify data entry, CONTAMW provides the ability to copy building component icons and to create data libraries that can be used in current and future modeling efforts. Some libraries are currently available in Persily and Ivy [2001].

Task 4 – Simulation

Simulation is the process of solving the system of equations assembled from a SketchPad representation of a building. This step requires the user to specify the type of analysis that is needed (steady-state, transient, or cyclical) along with many other simulation parameters. These parameters depend on the type of analysis desired and include weather data, convergence criteria, and in the case of a transient analysis, time steps, and the duration of the analysis.

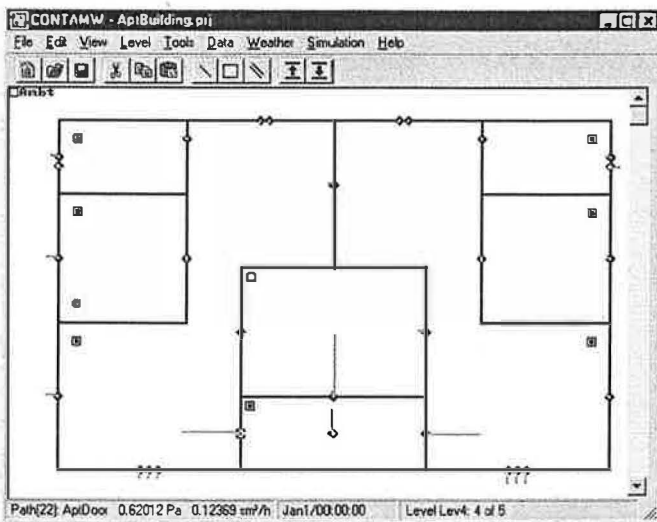


Figure 6: Graphical display of airflow (blue) and pressure difference (red) across airflow paths. Length of line indicates relative scale and value is displayed in the status bar.

Task 5 – Review & Record Results

Simulation results can be viewed on the screen and can be exported to a file for input to a spreadsheet program or other post processing software. Airflow and pressure differences at each airflow path can be viewed directly on the SketchPad (Figure 6). Contaminant concentrations can be plotted as a function of time (Figure 7). CONTAMW also provides a shaft report (Figure 8) that displays an elevation view of a building shaft along with pressure differences and airflow rates across two user-selected flow paths that connect the shaft zone to adjacent zones. This feature is useful in analyzing stairwell pressurization systems and viewing neutral pressure planes of a building.

Applications of CONTAMW

CONTAMW can calculate building airflows, which is useful in assessing building air change rates and interzonal airflow rates. It can also compare ventilation strategies. The pressure relationships between building zones are particularly useful in analyzing smoke control systems. The contaminant transport simulation capabilities can be useful for IAQ analysis including design, contaminant source isolation, IAQ investigations, and occupant exposure analysis. Following are some applications where CONTAMW can be useful. Where available, references to case studies that demonstrate the applicability of multizone modeling are included.

Calculate Building Air Change Rates

One of the main reasons for creating the CONTAM family of programs was to estimate building air change rates. Air change rates can be affected by a variety of driving forces including weather (wind and indoor-outdoor temperature difference) and mechanical ventilation system operation. CONTAMW provides the ability to establish sophisticated multizone building geometries, to simulate the effects of varying the driving forces on

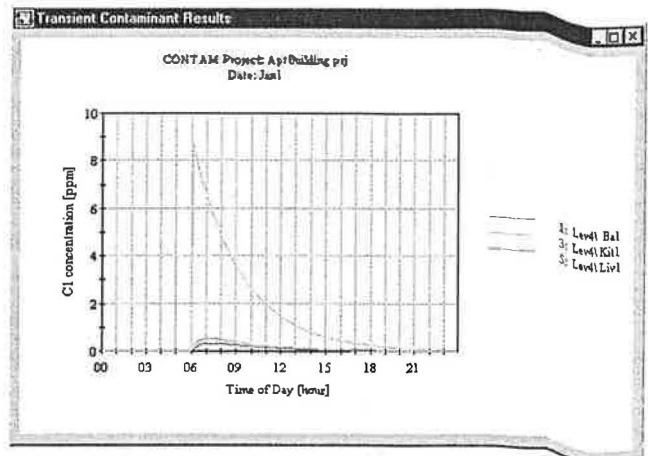


Figure 7: Contaminant simulation results as displayed by CONTAMW.

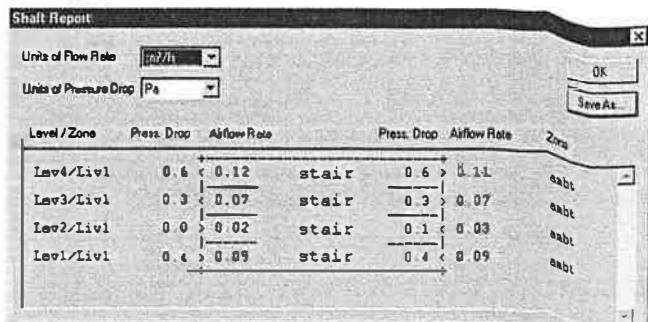


Figure 8: Shaft report shows direction of airflows from stairwell zone (stair) to apartment zone (Liv1) and outdoor zone (ambt).

building airflow, and to provide insight into the interactions of weather, envelope tightness, and air handling systems.

Building air change rates include airflow into a building both unintentionally through envelope leakage (infiltration) and intentionally by mechanical ventilation systems. CONTAMW accounts for each. Determining air infiltration rates can be useful in estimating energy impacts of building envelope leakage, understanding how weather affects infiltration, and analyzing the effectiveness of natural ventilation systems. Air change rate calculations can be useful in understanding the impacts of outdoor contaminant levels on indoor contaminant concentrations.

Analyze Ventilation Strategies

Along with the ability to analyze building air change rates, CONTAMW provides a rich set of tools to analyze ventilation strategies. Applications in this area include analyzing the effects of different ventilation strategies on IAQ and energy [Persily and Martin 1998; Emmerich and Persily 1998], sizing air handling systems, and analyzing natural ventilation systems and demand-controlled ventilation.

Compare Ventilation Strategies. A main strength of CONTAMW lies in its ability to analyze multiple scenarios for a given building geometry. Once that building geometry is established within a CONTAMW model, it can be reconfigured to

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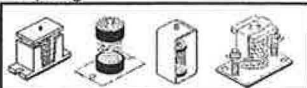
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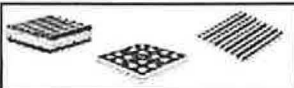
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investigate different ventilation strategies of interest. CONTAMW provides several ways to simulate mechanical ventilation systems including fixed flow-rate elements, a simple air handling system model, and a complex duct system model that can account for friction losses, duct leakage and air handlers as characterized by fan performance curves.

Design Natural Ventilation Systems. Multizone modeling has been used to design natural ventilation systems [Axley 1999]. CONTAMW can be used to investigate the differences in airflow rates obtained by varying different building features and weather conditions including the size and placement of ventilation openings in the building envelope, the orientation of the building to prevailing wind, the outdoor temperature difference and the size and location of ventilation stacks.

Demand Controlled Ventilation. Demand controlled ventilation (DCV) involves controlling ventilation rates based on monitored occupancy levels. Carbon dioxide (CO₂) can be monitored instead of monitoring occupancy levels directly because occupants are the dominant indoor source of CO₂. CONTAMW can be helpful in addressing issues related to the design and operation of DCV systems [Musser 2000]. Uses include analysis to determine levels of occupant and non-occupant related contaminants that might result.

Building Flush Out. Buildup of non-occupant related contaminants is a concern with DCV or any ventilation system that reduces or shuts off ventilation during unoccupied hours. CONTAMW can be useful in analyzing contaminant buildup in those situations and in determining the amount of ventilation required to purge, or flush out, the contaminants prior to occupancy [Musser 2000].

Analyze Contaminant Transport

As the name suggests, CONTAMW simplifies the analysis of airborne contaminant transport within complex, multizone buildings. Contaminant behavior within buildings can be influenced by airflow, source and sink properties, particle filtration, gaseous air cleaning, and chemical reactions. CONTAMW provides the ability to address all of these mechanisms, making it useful in understanding many contaminant-related building issues and solving or preventing contaminant-related problems in the built environment.

Predicting contaminant concentrations can be used to determine indoor air quality performance before a building is constructed and occupied, to investigate the impacts of ventilation system design decisions and building material selection, and to assess the indoor air quality performance of an existing building. Predicted contaminant concentrations can also be used to estimate personal exposure based on occupancy patterns in a building [Persily 1998].

IAQ Design

Designers typically deal with IAQ by specifying minimum outdoor air ventilation rates on a space or whole building level using requirements in building codes or standards. The Ventilation Rate Procedure in ASHRAE Standard 62-1999 is a prescriptive approach that provides minimum ventilation requirements [ASHRAE 1999]. Standard 62 also contains a perfor-

mance-based IAQ Procedure that addresses IAQ through maintaining acceptable levels of known contaminants. CONTAMW can be useful in implementing both of these procedures from the point of view of ventilation system and building material impacts. CONTAMW can also account for outdoor air contaminant levels, the use of filtration, consideration of intermittent or variable occupancy, and distribution of ventilation air to multiple spaces.

Contaminant Source Isolation

Contaminant source isolation refers to preventing contaminant transport from one zone into another. Examples include parking garages, toilets, and radon entry from the soil [Fang and Persily 1995]. These situations involve establishing airflow or pressure differentials between different zones of a building to control contaminant migration. The ability to use CONTAMW to define complicated multizone systems enables the analysis of contaminant transport not only between adjacent zones, but also through less obvious paths via elevator and stair shafts, service chases, and duct leakage.

Design of Smoke Management Systems

Smoke management refers to passive and active control of smoke movement within the built environment in the interest of providing safety to occupants, firefighters, and property. Smoke management methods include *compartmentation, dilution, pressurization, airflow, and buoyancy* [Klote and Milke 1992]. CONTAMW has been used to analyze the performance of many of these techniques. It has been used to simulate smoke movement in multizone facilities, to analyze the performance of smoke control systems including stairwell pressurization systems, and to aid in performing far-field tenability (occupant safety) analysis [Ferreira 1998].

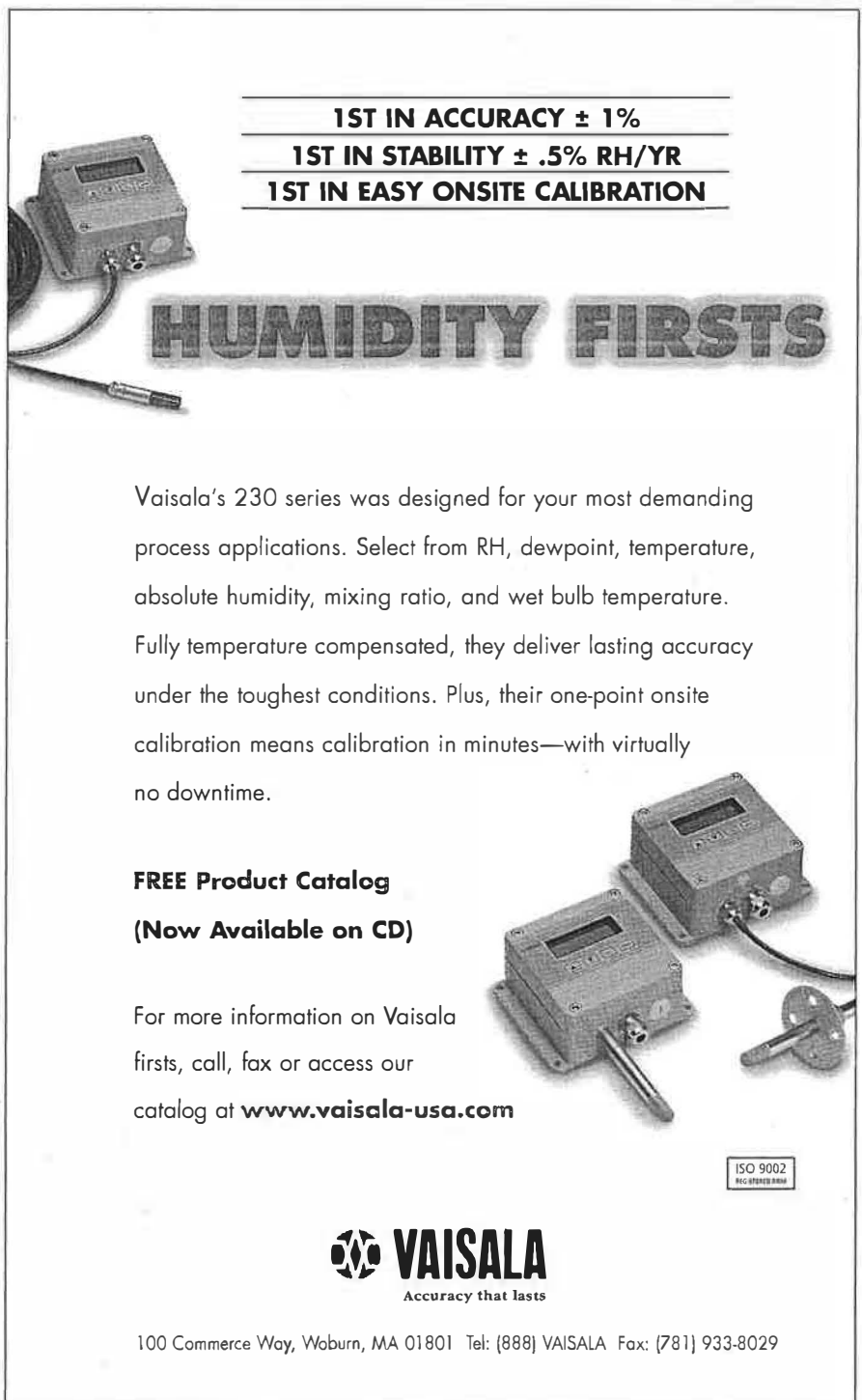
Summary

CONTAMW is a useful tool for analyzing airflow and contaminant transport in complex multizone buildings on a macro level. This article is only an introduction to the program's capabilities and does not cover all the capabilities, options and ap-

plications. The capabilities of multizone modeling are continually being extended, and many creative engineers are applying them in new ways.

CONTAMW is available in the public domain free of charge by download from NIST's Building and Fire Research Laboratory web site at www.bfrl.nist.gov/863/

contam. The project file used for this article also is available for download at this site. NIST is developing a web site that will provide support in the form of CONTAMW building component data libraries, post-processing software, and multizone modeling case studies and references at www.bfrl.nist.gov/iMZWeb.



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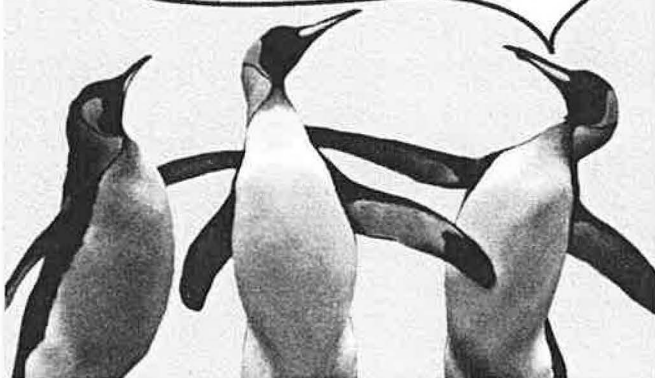
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