

# A SOFTWARE TOOL FOR ANALYZING BUILDING AIRFLOW AND AIRBORNE CBR AGENT CONCENTRATIONS

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*Contaminant concentrations that result within buildings in response to airborne chemical, biological and radiological (CBR) events are due to a complex interaction between the building construction, ventilation system performance and weather conditions. The analysis of such events requires a tool that can address this complex interaction on a whole-building scale. CONTAM is a public domain multizone airflow and contaminant transport software tool developed by the National Institute of Standards and Technology. CONTAM provides the ability to define building models that capture the multizone nature of building airflows including the impacts of ventilation systems, contaminant source and removal mechanisms, and weather conditions. The program has been applied over the past decade for both design and analysis of building systems in the areas of indoor air quality, building ventilation, smoke management, and more recently, CBR-related events. This paper will present an overview of the CONTAM program and its applicability to building-related CBR events.*

## I. INTRODUCTION

People spend a large portion of their time within buildings, which provides a motivation to understand occupant exposure to potentially hazardous airborne contaminants. Sources of these potential hazards range from those generated indoors by building materials, furnishings and occupant-related processes as well those generated outdoors. Both indoor and outdoor sources can include chemical, biological and radiological (CBR) releases, whether accidental or purposeful.

Contaminant transport within buildings involves a complex interaction between building construction and layout, mechanical and natural driving forces, and chemical transport mechanisms. There are a variety of modeling approaches and tools aimed at capturing these complex interactions. One means of categorizing these tools is by the level at which they resolve the spatial

domain (airflow field) of a building from the more detailed (micro-scale) to the less detailed (macro-scale).

At the micro end of the scale is the class of models referred to as computational fluid dynamics (CFD), at the macro end is the multizone or nodal class, and the zonal class of models is in between. The fine resolution of CFD lends itself very well to addressing detailed variations within a room (e.g., pressure, velocity and contaminant concentration), but this fine resolution also leads to a large set of equations to be solved which in turn requires significant computational time. In contrast, multizone models<sup>[1-4]</sup> generally treat each room as a single zone whose properties do not vary spatially within the zone. This leads to the ability to address the entire building domain, but in less detail.

CONTAM is a multizone modeling tool that was originally developed to address indoor air quality and building ventilation issues on relatively large spatial (i.e., whole building) and long temporal (days, weeks and months) scales. Its ability to determine interzone pressure relationships within buildings has led to its wide spread use in analyzing and designing smoke management systems<sup>[5, 6]</sup>. More recently, CONTAM has been applied in the area of CBR analysis. This area of application is driving development of CONTAM to address more acute events which tend to require finer spatial and temporal scales.

## II. CONTAM

CONTAM is public domain software that can be obtained from the National Institute of Standards and Technology (NIST) website<sup>[7]</sup>, along with other support software and documentation. CONTAM consists of two main components: the graphical user interface ContamW and the simulation engine ContamX. ContamW is a Windows application that implements an icon-based SketchPad used to develop schematic representations of buildings in plan view. As described by Lorenzetti, “the schematic is used to idealize a building as a network of

discrete flow elements such as doors, cracks, and ductwork. The flow elements connect at nodes, which represent either static zones such as rooms, or points where two elements meet, such as duct junctions. The governing equations represent: (1) pressure–flow relations in the flow elements, (2) mass conservation at the nodes, and (3) hydrostatic pressure variations in the zones.<sup>[8]</sup> SketchPad representations are not to scale, but the topology of the zones is important in providing interzone connectivity. The development of these *idealizations* is an important aspect of performing multizone analysis to ensure useful simulations are performed to accomplish the goals of the analysis<sup>[9-11]</sup>. A sample SketchPad is shown in Fig. 1.

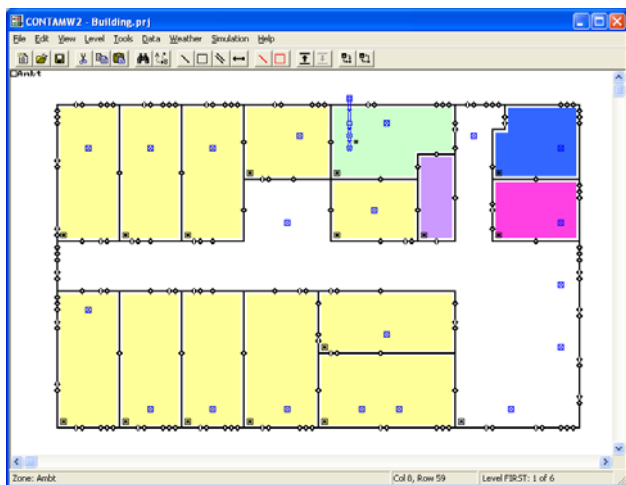


Fig. 1. Example schematic floor plan representation as implemented with the ContamW SketchPad.

### Program Inputs

ContamW provides for the input of multiple building *levels* including plenums and multi-floor zones such as atria. Walls that make up the *zones* are drawn by the user, and *airflow paths* (doors, windows and other leaks) are placed on the walls and floors to provide connectivity between adjacent zones. Ventilation systems can be defined using either a *simple air handling system* or a detailed *duct* model. Contaminant *sources* and *sinks* (removal mechanisms) can be placed within individual zones and filters can be placed within the ventilation system. *Occupants* can be placed within the building and scheduled to move about, thereby allowing the calculation of their exposure over time. A set of *building control* elements including sensors and a range of mathematical and logical operators enables the creation of control networks that can modulate fans, dampers and other elements based on contaminant concentrations, interzone pressure differences or air temperatures. Both *weather* and *ambient contaminants* can be defined using

associated input files. ContamW also provides for the input of parameters to control ContamX calculations.

### Calculations Performed

ContamX uses the building description as input via ContamW to establish a set of mass balance equations for each airflow node (zones and duct junctions) and solves the resultant set of non-linear algebraic equations for the zone pressures that satisfy the mass balance equations. Once the airflows have been determined, the contaminant calculations are performed by solving a linear set of differential equations based on a finite difference formulation of the mass balance equations for each contaminant. Calculation details are provided in the CONTAM user manual and related documentation<sup>[1, 8]</sup>.

ContamX provides the ability to perform steady state simulations or transient (quasi-steady) analyses for up to one year at time steps ranging from one second to one hour. Contaminant calculations can be either implicit or fully explicit using the recently developed *short time step method* that includes the ability to simulate one-dimensional convection/diffusion within the detailed duct system and zones designated as one-dimensional otherwise all zones are considered to be *well-mixed*, i.e., characterized by a single contaminant concentration throughout the zone.

Specialized methods also enable the simulation of whole building pressurization tests and duct balancing. Another simulation option outputs key airflow characteristics of a building that are useful in evaluating the reasonableness of a building model.

### Program Outputs

Outputs of ContamX include zone pressures, airflow rates and pressure differences across airflow paths, whole building air change rates, zone contaminant concentrations, occupant exposure levels and filter loading reports. These outputs are stored in simulation results files that contain either steady state values or transient time histories of results depending on the type of simulation performed.

ContamW provides the means to review results via the SketchPad. SketchPad results include scaled, directional pressure difference and airflow indicators, a floating toolbar that displays zone and duct system gage pressures as well as a results display window that provides detailed zone concentrations and airflow summaries for the user-selectable result time.

Graphs of contaminant, airflow and pressure difference time histories can be generated from within ContamW or data can be exported for further analysis, e.g., via spreadsheet programs. The results viewing program, ContamRV, provides color-coded SketchPad display of contaminant and zone pressures.

## General Applications

These features combine to enable a wide variety of building analyses. Pressure calculations provide the means to evaluate relative pressurization between building zones which is applicable to smoke management systems and isolating spaces when spaces used for different purposes are mixed together within a given building, for example in cases of health care, laboratory and material handling facilities. One such example in which CONTAM is being used is in nuclear material handling facilities to ensure that the building system as a whole has balanced airflows and that space exhaust systems function as intended<sup>[12]</sup>. Relative pressurization also pertains to shelter-in-place locations and strategies as that may be employed in response to CBR events. Ventilation system airflow modeling enables the analysis of various ventilation systems and strategies as they relate to energy use, indoor air quality and system response to CBR events<sup>[13]</sup>. Contaminant transport and occupant exposure calculations provide for the evaluation of various contaminant emission and removal mechanisms including filtration as they pertain to indoor air quality and occupant exposure thresholds. These features are also useful in evaluating exposure levels during CBR events.

## III. APPLICATION TO CBR

In general building airflow and contaminant transport modeling is applicable to CBR analysis in the areas of system design and retrofit, operational planning and research. Building system design includes those aspects of the building system that affect ventilation and contaminant transport, e.g., ventilation system airflow rates, contaminant filtration and building envelope leakage. Operational planning refers to those aspects that pertain to system response to events such as building sensor and control strategies or shelter-in-place usage. Research is ongoing in the development of the analysis capabilities themselves and their application to building protection.

One of CONTAM's strengths is its ability to perform a large number of simulations in a relatively short amount of time. This along with its ability to consider the building and ventilation system as an integrated whole enables the simulation of different building and system configurations, operating strategies and agent release scenarios with relative ease and in virtually limitless combinations.

### System Design and Retrofit

While CONTAM is not a design tool in the strictest sense, its relatively straightforward learning curve and quick calculation speed enables the performance of what-

if scenarios that make it suitable as a design tool. It can be useful in making decisions related to: building layout, ventilation system design, filter selection, building pressurization, and building envelope tightness that can be subsequently used to perform life-cycle cost analysis.

Building layout decisions include the relative placement of building zones according to space use as well as the placement of ventilation system outdoor air intakes and return air points. The effects of indoor sources as they relate to nearby spaces can be evaluated. For example, the location of spaces that might be more vulnerable to indoor releases such as lobbies, meeting rooms and mailrooms can be easily investigated by placing CONTAM's indoor sources in these zones and evaluating the transport to other occupied zones such as offices.

Outdoor air intakes into mechanical ventilation systems are potential points of vulnerability. CONTAM allows one to study location of such intakes in relation to outdoor contaminant releases in two ways. Ambient contaminant files enable the definition of a *global* ambient or outdoor contaminant concentration that does not vary spatially but can vary with time (CTM file). Alternatively, one can employ a more detailed contaminant file that can vary ambient concentrations both spatially and temporally (WPC file). The WPC file can be generated based on separate CFD analysis of a building's surroundings using exterior plume and dispersion models for various outdoor sources.

Short of preventing an agent release, filtration can be a very effective building protection strategy<sup>[13,14]</sup>, assuming the filtration media is effective at filtering the agent in question. CONTAM provides multiple filter models including simple constant efficiency models, particle size-based models that can be used to represent filters based on filter rating curves<sup>[15,16]</sup> (see Fig. 2) and gaseous contaminant models that are a function of filter loading. Filters can be placed within the outdoor, supply, return and recirculation points of the mechanical ventilation systems making it very easy to compare different filtration strategies for a given mechanical configuration. Filters can also be used to simulate portable filtration devices located within or dedicated to filtering a specific room or area of a building. Filter loading reports are provided for each simulation. These reports provide the total mass of contaminant that the filter is challenged with and the total mass removed by the filter.

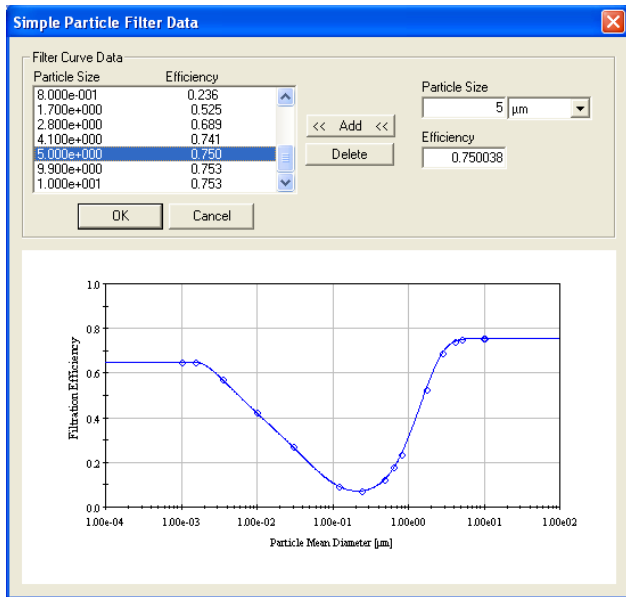


Fig. 2. Particle filter model of a MERV 11 filter.

Perhaps one of the more common applications of CONTAM concerns the analysis of building pressurization strategies. An example of such an application is the design of pressurization systems for smoke management purposes. The same principles can be applied to the relative pressurization of spaces to one another for purposes of reducing the risk of contaminant transport between various zones of a building. CONTAM accounts for the pressures induced by both the mechanical ventilation system operation as well as interzone airflows induced by outdoor weather conditions. This unique capability provides the means to virtually balance interzone airflows to achieve desired pressure relationships. Ventilation systems airflows can be easily adjusted along with interzone leakages, e.g., door opening, undercut and transom area, to investigate various building configurations. Some specific applications of this relative pressurization technique include selection and design of rooms to be used for shelter-in-place strategies and design of mailroom isolation systems. These applications can also include the filter modeling capabilities as previously mentioned.

Pressurization not only refers to interzone relationships, but also the relationship between the interior and exterior of a building across the building envelope. CONTAM enables the simulation of building pressurization tests<sup>[17]</sup> to gauge the envelope leakage<sup>[18]</sup>. Once the leakage characteristics of a building envelope are defined in CONTAM, it can be used to calculate pressure differences across the envelope under various weather and ventilation system operating conditions. Weather affects envelope pressures via wind speed and direction and indoor – outdoor air temperature differences

that can induce the so-called stack effect<sup>[19]</sup>. Building pressurization can be used as a means to control the transport of contaminants through leaks in the building envelope in the event of an outdoor agent release. However, the effectiveness of a mechanical system to pressurize a building is highly dependent on envelope air tightness<sup>[20]</sup>. The infiltration that can occur as a result of envelope leakage can reduce the effectiveness of filtration of the purposeful outdoor air intake via the mechanical system, and CONTAM enables the evaluation of these effects.

## Operational Planning

Response to CBR-related events involves planning the operation of the building systems during various phases of an event – before, during and after; to protect the occupants, accommodate first responders and decontaminate the building. Prior to an event, the building should be designed so that the building is configured and systems are in place in order to affect the desired operations during an event. The previous section addressed the various elements of building design that can be addressed using CONTAM. This section will focus on the next two phases of operational planning.

During an event one of the main concerns is how, if at all, the ventilation system should be operated. Questions arise as to whether air handlers should be turned off, left on, adjusted to achieve relative pressurization strategies (as might be done with smoke management systems), as well as the timing of such adjustments. Some have suggested operational strategies that would be activated automatically based on agent sensors. Real-time operational changes in response to a CBR release raise a complex set of issues that is always building, system and event specific. CONTAM provides the ability to analyze various strategies for specific buildings and release scenarios to determine desirable courses of action. Fig. 3 shows examples of various operational protection strategies for a hypothetical building compared with design-based filtration strategies<sup>[13]</sup>. For the cases investigated, the figure reveals the reduction of contaminant concentrations inside the building by filtration strategies and that shutdown procedures can actually increase occupant exposure by varying degrees depending on the timing of the shutdown.

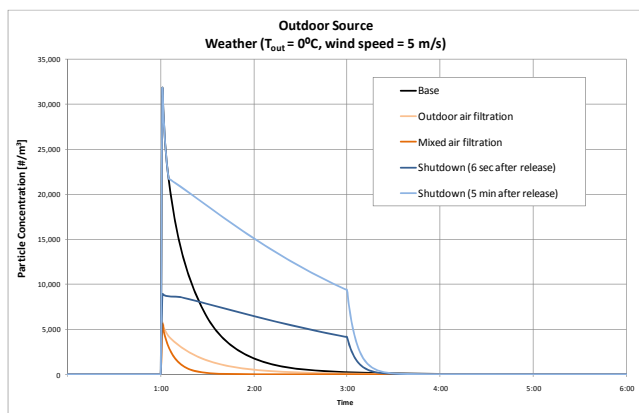


Fig. 3. Chart showing comparison between filtration and fan shutdown protection strategies for a hypothetical highrise building influenced by weather conditions.

During an event, first responders may play several roles in building protection including building evacuation and adjustment of system operation, for example, to purge contaminants from the building. CONTAM can be useful in helping first responders and building managers to develop evacuation plans and system adjustment strategies in response to specific events identified in the planning phase. These strategies can include the designation of shelter-in-place locations and duration of sheltering. Scenarios and response strategies can be explored with building operators and first responders as a training tool. One such application has been implemented within the Advanced Combat and Tactical Simulation<sup>[21]</sup> (ACATS) tool using CONTAM's real-time communications ability to integrate it as a component of the simulation system.

CONTAM simulations can also be used to evaluate levels of contaminant concentrations that may have occurred within a building as a result of an event and assist in developing decontamination strategies for the building. It could be used to simulate the dispersion of a decontamination agent within a building to determine adequate levels of the agent are attained as well as the clearing of the agent at the end of the decontamination process.

## Research

Multizone modeling is useful in many aspects of building research, and multizone modeling itself is an evolving topic of research. Multizone modeling research as it applies to building protection falls into two basic categories: analysis of protection strategies and model development.

CONTAM has been under development for the past two decades<sup>[22]</sup> and has continuously evolved to address a wider range of applications including building protection.

As presented in the previous section, it is being used to analyze a range of protection strategies. Multizone modeling is also being implemented to evaluate other building protection issues such as sensor placement, first responder training, and post-event contaminant sampling location selection strategies.

Multizone models have been used to analyze sensor placement and source location strategies within buildings<sup>[23-26]</sup>. The models provide a means to develop large datasets that contain the results of multiple simulations of different release, building configuration, ventilation system operation, and weather scenarios in combinations that would be otherwise impractical to obtain experimentally. Similarly, multizone models are being used to analyze and develop sampling strategies for determining contamination levels after CBR events and subsequent building decontamination.

Methods to develop evacuation plans and "safe" routes through a building during or soon after an event are also being investigated using multizone modeling. The models are utilized two ways: as a virtual building in place of experimental measurements and as a component of a route-planning system to predict contaminant transport during an event. In the latter application, building controls are adjusted as part of an intelligent building environmental system used to establish safe routes<sup>[27]</sup>.

The use of CONTAM as an integral part of a real-time building protection system is being investigated in combination with outdoor contaminant transport models, sensor arrays and building energy management systems<sup>[28]</sup>. Such systems will enable training much like the ACATS system mentioned above, but extend the concept by utilizing it during events to predict contaminant transport based on real-time indoor and outdoor sensor readings, current building configuration (open/closed doors etc.) and system operations, and selected response strategies. Such systems could also implement a safe-route component as described previously.

The development of the multizone models themselves is a subject of research to further improve their ability to capture the physics of mass transport phenomenon, the availability of reliable input parameters, and general usability. There are many aspects of CONTAM that could be improved; some of the more immediate needs relevant to CBR are mentioned here. This is not an exhaustive list and others have addressed shortcomings of multizone models and ways to improve them<sup>[29-31]</sup>.

Mass transport analysis enhancements include the following: improved aerosol transport models, a broader set of filter models, robust methods to handle combined heat transfer and airflow, moisture transport, and particle deposition within ducts. Some of these features may be available as a stand-alone tool or in a simpler form that

could be integrated into a multizone tool. In some cases the phenomenon themselves are quite complex and difficult to capture in a comprehensive form, so trade-offs must be made to implement them based on current understanding. An example of the latter is modeling of particle deposition/resuspension with respect to building surfaces<sup>[32, 33]</sup>.

Implementing features within a tool does not in and of itself render that feature useful. Input parameters are often lacking for models that are empirical or that are based on first principles. For example, some contaminant source models that are implemented within CONTAM were based on data obtained from emission chamber characterization measurements and fitted to an empirical equation. These inputs are not necessarily going to be relevant to other sources. Further, data may exist but not be readily available or in a format that is immediately usable within the tool. Some efforts have been made to improve upon this situation<sup>[34]</sup>.

In terms of general usability, the desire to capture the intra-zone details of contaminant and airflow fields within perhaps a select zone (or few) of interest is a major topic of research. Specifically, the integration of CFD models with multizone models is being investigated<sup>[35-37]</sup>. CONTAM has recently implemented a relatively simple one-dimensional convection/diffusion calculation that captures contaminant diffusion along a user-specified axis or within an entire duct system<sup>[1]</sup>.

#### IV. CONCLUSIONS

Multizone modeling is a useful tool to include in a toolbox for developing and analyzing strategies to better protect buildings from airborne CBR events. Other tools in this arsenal include physical security, hardening of buildings, human factors, CBR contaminant detection and filtration, and operation and maintenance of the building ventilation system.

When using multizone modeling, the model assumptions must be kept in mind, especially the well-mixed zone and lack of momentum effects. CONTAM is not the only multizone analysis tool available and others may handle some aspects that CONTAM does not, however, there are trade-offs among all of the available tools. CONTAM's strong suits are its flexibility, relative ease in developing building-specific models and the speed and robustness of its simulation engine. While it is desirable to enhance the tool with as many useful features as possible, it is also desirable to maintain these important features in the process.

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