Development and Application of an Updated Whole-Building Coupled Thermal, Airflow, and Contaminant Transport Simulation Program (TRNSYS/CONTAM)

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Abstract

The TRNSYS energy analysis tool has been capable of simulating whole building coupled heat transfer and building airflow for about ten years. The most recent implementation was based on two TRNSYS modules Type 56 and Type 97. Type 97 is based on a subset of the airflow calculation capabilities of the CONTAM multizone airflow and contaminant transport program developed by the National Institute of Standards and Technology (NIST). This paper describes the development of new CONTAM capabilities in support of an updated combined, multizone building heat transfer, airflow and contaminant transport simulation approach using TRNSYS. It presents an illustrative case that highlights the new coupling capability and also presents the application of this coupled simulation approach to a practical design problem of the energy use related to airflow through entry doors in non-residential buildings.

Keywords: building simulation; CONTAM; coupled thermal, airflow and contaminant modeling; multizone modeling; TRNSYS

1. Introduction

High performance buildings must meet demanding energy and indoor air quality (IAQ) requirements through the use of innovative building designs and technologies for ventilation and IAQ control, such as natural ventilation and demand controlled ventilation (DCV) (Persily and Emmerich 2012). Modeling and simulation tools improve the abilities of designers to achieve coordinated and integrated systems. Passive design features (i.e. the architectural and envelope aspects) can be optimized to reduce the need for designs that implement active strategies (i.e., HVAC systems) for thermal conditioning. Source control can be implemented as a fundamental approach to reducing contaminant levels inside buildings thus reducing the need for removal via ventilation and air cleaning. Due to interactions between building temperatures, airflows and contaminant concentrations, the design and analysis of these buildings and systems require advanced modeling capabilities to simultaneously account for these transport phenomena.

Class of Models

We address the class of whole-building multizone (or nodal) simulation tools that implement energy and mass conservation mathematical models of heat transfer, airflow and contaminant mass transport in the form of non-linear ordinary differential equations (ODEs) on a so-called macro-scale. The multizone aspect of the models refer to the treatment of building zones as well-mixed volumes of air whereby, for the purposes of simulation, a building is segmented on thermal zone or room airflow boundaries depending on the simulation regime in question, e.g., building energy or inter-zone airflow and contaminant transport. In particular we concern ourselves with the TRNSYS (Klein et al. 2012) energy simulation and CONTAM (Walton and Dols 2005) airflow and contaminant transport analysis tools.

Mathematical Models

The heat transfer equations are reformulated as linearized ODEs and differential algebraic equations (DAE) in order to take advantage of linear solution techniques to solve the associated initial value problems. This approach to formulating the heat balance among the building air volumes and surfaces is presented in Chapter 18 of (ASHRAE 2013) and (Schneider, Roux, and Brau 1995) and the mathematical description of the TRNSYS multizone heat transfer building model (Type 56) is provided in Volume 5 of (Klein et al. 2012).

The CONTAM airflow calculations are based on non-linear airflow-vs-pressure relationships as presented in (Walton and Dols 2005). These relationships are referred to as power-law airflow elements e.g., the orifice flow equation. Lorenzetti provides a detailed treatment of the computational aspects of the Newton-Raphson solution technique used to determine the nodal pressures that provide the mass balance of the multizone airflow problem (Lorenzetti 2002).

CONTAM provides several methods of solving the contaminant mass balance equations. These methods are referred to as:

- default solver (implicit/semi-implicit Euler)
- short-time step (STS) solver (explicit Euler)
- CVODE solver (stiff, general ODE solver)

The default solver implements an implicit Euler method (backward difference) by which the contaminant mass balance equations are reformulated as a set of DAEs that can be solved using a number of available linear solution techniques (Walton and Dols 2005). This default solver has also been coupled with the computational fluid dynamics, zero-equation turbulence model solver (CFD0) to capture the within-zone variations of airflow and contaminant concentrations (Wang and Chen 2007; Wang 2008; Wang, Dols, and Chen 2010). The STS solver employs an explicit Euler method (forward difference) to directly solve the DAEs as well as allowing for the treatment of one-dimensional convection-diffusion within designated zones, e.g., long hallways, and ducts. Lorenzetti, et al. present the general-purpose solution technique for ODEs as implemented by the CVODE solver that has recently been implemented within CONTAM to better handle mass transport process the can lead to stiff contaminant mass balance equations, e.g., chemical sorption and reactions (Lorenzetti et al. 2013).

Coupling Approaches

Separately, these modeling regimes have been addressed by well-established simulation tools implementing various modeling assumptions that enable them to address a wide range of design and analysis problems (Walton and Dols 2005; Feustel 1999; Crawley et al. 2001; Klein et al. 2012). However, treating these regimes separately fails to properly account for the interactions between coupling transport variables, e.g., temperature and airflow. Addressing the interaction among all three of these simulation regimes requires either a fully integrated/simultaneous solution method or the use of coupled simulation whereby regimes are solved by there respective methods and data is exchanged between the co-dependent regimes.

Coupling can be accomplished using various methods. Program modules, e.g., heat transfer and airflow, can be tightly coupled whereby iteration and data exchange between them can be closely monitored and step-wise adjustments or relaxation factors can be applied to control solution oscillation. This tight coupling requires direct access to and modification of the program code. Modeling regimes can also be loosely coupled using co-simulation techniques whereby the solution of each regime is handled separately, and the exchange of data is coordinated according to pre-arranged methods of interfacing the subsystems or programs (Nouidui, Wetter, and Zuo 2013). These methods of co-simulation can be performed using either *dynamic* or *quasi-dynamic* coupling sometimes referred to in the combined heat transfer and airflow simulation community as “onion” or “ping-pong” coupling (Hensen 1995). These methods benefit from the use of existing simulation tools that can be well-characterized for the regimes at which they are targeted; however, they can exhibit stability issues that can lead to difficulties in obtaining robust, reliable and accurate solutions in the coupled domain (Arnold, Clauss, and Schierz 2013). Although, the tools must be modified to enable the inter-process communication according to the agreed upon data exchange method, once this has been accomplished the tools become more accessible via the coupling framework thus allowing further study of the application of these tools within coupling frameworks such as TRNSYS, functional mockup interface (FMI) or OpenPALM (MODELISAR 2010; Morel et al. 2013).

Clarke presents a comprehensive overview of how to address the interaction of energy and airflow, the various mathematical models associated with these regimes, the full matrix formulations and numerical techniques that can be used to treat them as fully interactive and dynamic regimes as well as potential difficulties involved with these techniques (Clarke 2001). Wang et al. develop and demonstrate simultaneous and semi-simultaneous solution methods on a natural ventilation case that reveals promising results without the need to apply solution stabilization techniques that may be required when utilizing loose coupling methods (Wang, Dols, and Emmerich 2012).

Numerical solutions of ventilation airflow rates and temperatures of room air and wall assemblies have long been treated separately. Multizone airflow network models, such as CONTAM (Walton and Dols 2005), COMIS (Feustel 1999) and others predict building airflows without solving the energy equation. As a result, air temperatures are required to be provided for each zone (or room). On the other hand, building energy analysis software tools are often not developed to determine inter-zone airflows as a multizone network model does. Over the past two decades, several efforts have been conducted to integrate building airflow network models with building energy analysis tools. Huang et al. linked COMIS 3.0 with the EnergyPlus building energy simulation program (Crawley et al. 2001; Huang et al. 1999), Dorer and Weber developed the COMV-TRNS module for TRNSYS (Dorer and Weber 1999), and in 2003 TRNFlow was developed to link COMIS with TRNSYS (Weber et al. 2003). Walton developed a coupled thermal and airflow simulation tool that was demonstrated for modeling a commercial building with both natural and hybrid ventilation (Axley, Emmerich, and Walton 2002). McDowell et al. integrated CONTAM with the TRNSYS building energy simulation software package (McDowell et al. 2003; Klein et al. 2012). Gu added an airflow network model to EnergyPlus and showed some encouraging results (Gu 2007). Another popular energy simulation package with its own airflow models is the Environmental Systems Performance, Research version (ESP-r) building simulation program (Clarke 2001).

2. Updated TRNSYS/CONTAM coupling approach

TRNSYS is a **TR**a**N**sient **SY**stems **S**imulation program with a modular structure that enables multiple energy-related systems to be considered together within a single simulation environment (Duffy et al. 2009). Modules are referred to as Types. TRNSYS includes many Types and allows users to develop custom Types for their purposes. Version 17 includes two types that allow for the simulation of multizone building heat transfer and airflow, Type 56 and Type 97, respectively (McDowell et al. 2003). Type 97 is based on a subset of capabilities of the multizone airflow and contaminant transport program CONTAM (Dols 2001; Walton and Dols 2005; Wang, Dols, and Chen 2010), developed by the National Institute of Standards and Technology (NIST). This subset includes the ability to model inter-zone airflows based on a limited number of the mathematical airflow elements that exist in CONTAM and to use the simple air handling system model available in CONTAM. This coupling was done using the dynamic coupling approach (Hensen 1995), whereby iteration occurs between the modules within each time step until convergence is obtained and then the simulation proceeds to the next time step. Aside from the aforementioned stability issues associated with the dynamic coupling approach, there are several limitations to the previous coupling method via Type 97 including:

- no contaminant transport modeling,
- does not utilize the full duct model of CONTAM,
- connections with Type 56 are not formed automatically , and
- does not “evolve” with new versions of CONTAM as it is continuously enhanced by NIST.

NIST has addressed these limitations by developing a method and a new TRNSYS Type 98 to more fully couple the actual simulation engine of CONTAM (referred to as ContamX) with TRNSYS.

This updated coupling approach between TRNSYS and CONTAM consists of several software tools but is centered on the new Type 98. This type utilizes the existing socket communication capabilities and data transfer messages of ContamX to provide for the exchange of data between ContamX and Type 56 via the TRNSYS simulation engine. The coupling between the heat transfer and airflow calculations is accomplished via the quasi-dynamic method as opposed to the dynamic method. The quasi-dynamic, or loose coupling (Zhai and Chen 2005; Trcka, Wetter, and Hensen 2009), refers to the coupling between simultaneously running processes whereby data is exchanged only once within each time step, and convergence only occurs within each process, i.e., not between the processes. For example, the airflow calculation process determines inter-zone airflow rates at time *t*, passes them to the heat transfer calculation process, which then determines the temperatures at time *t*. These temperatures are then used by the airflow process when it calculates values for time $t+\Delta t$, and so on. TRNSYS provides the ability to select with which process to begin, i.e., heat transfer or airflow. Inter-process convergence under the dynamic coupling method can be more difficult to achieve than with the quasi-dynamic method. However, the quasi-dynamic method will benefit from and may require the use of shorter time steps than would be usable under non-coupled circumstances (Hensen 1995).

In order to improve coordination of the exchange of data between the two Types, NIST modified the CONTAM graphical user interface (referred to as ContamW), and developed additional software tools to support a process to perform this coordination. Specifically, ContamW was modified to provide for scaled drawing of building floor plans (within the rectilinear confines of the existing program). The *CONTAM3DExport* tool was also developed to “extrude” a CONTAM sketch into a three-dimensional file (IDF file) that can be imported into *Trnsys3d*. Another utility, the *Type56-98Coupler*, aids in generating the associated *proforma* that defines the inputs and outputs of Type98 and in forming the links between the inputs and outputs of Type 56.

Illustrative example

The following example provides an overview of the coupling process and capabilities. This case provides thermal/airflow coupling, coordination of heating, ventilating and air-conditioning (HVAC) air-handling equipment, and contaminant calculations for a CO_2-based DCV system with a heat recovery ventilator (HRV). A scale CONTAM model of a small, hypothetical house with one floor and an attic was developed in ContamW as shown in Figure 1. This was extruded to a 3D IDF file and modified to establish a gable roof and shading on the front of the building as shown in Figure 2.

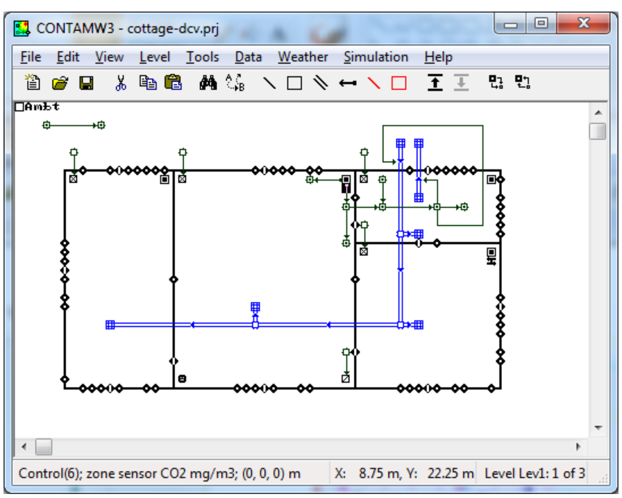


Figure 1. CONTAM SketchPad of small house

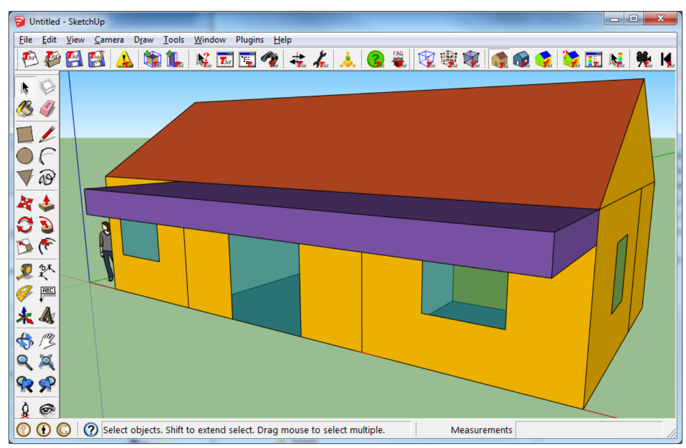


Figure 2. Trnsys3d model of small house

The resultant IDF file was then imported into *TRNSYS Simulation Studio* as a new 3D Building Project (multizone). The project was then coupled using the *Type56-98Coupler*. The coupler creates inputs and outputs for Types 56 and 98 as provided in Figure 3 and establishes connectivity between the two Types based on the CONTAM project file. Figure 3 shows the inputs and outputs of the TRNSYS Types and their connectivity. The red text and lines in Figure 3 indicate the inputs, outputs and connections that are automatically created during the coupling process, and the blue lines indicate user-defined connections made within the TRNSYS Simulation Studio. The heating, cooling and HRV systems were added within the TRNSYS Simulation Studio to obtain the resulting project with interconnected Types as shown in Figure 4.

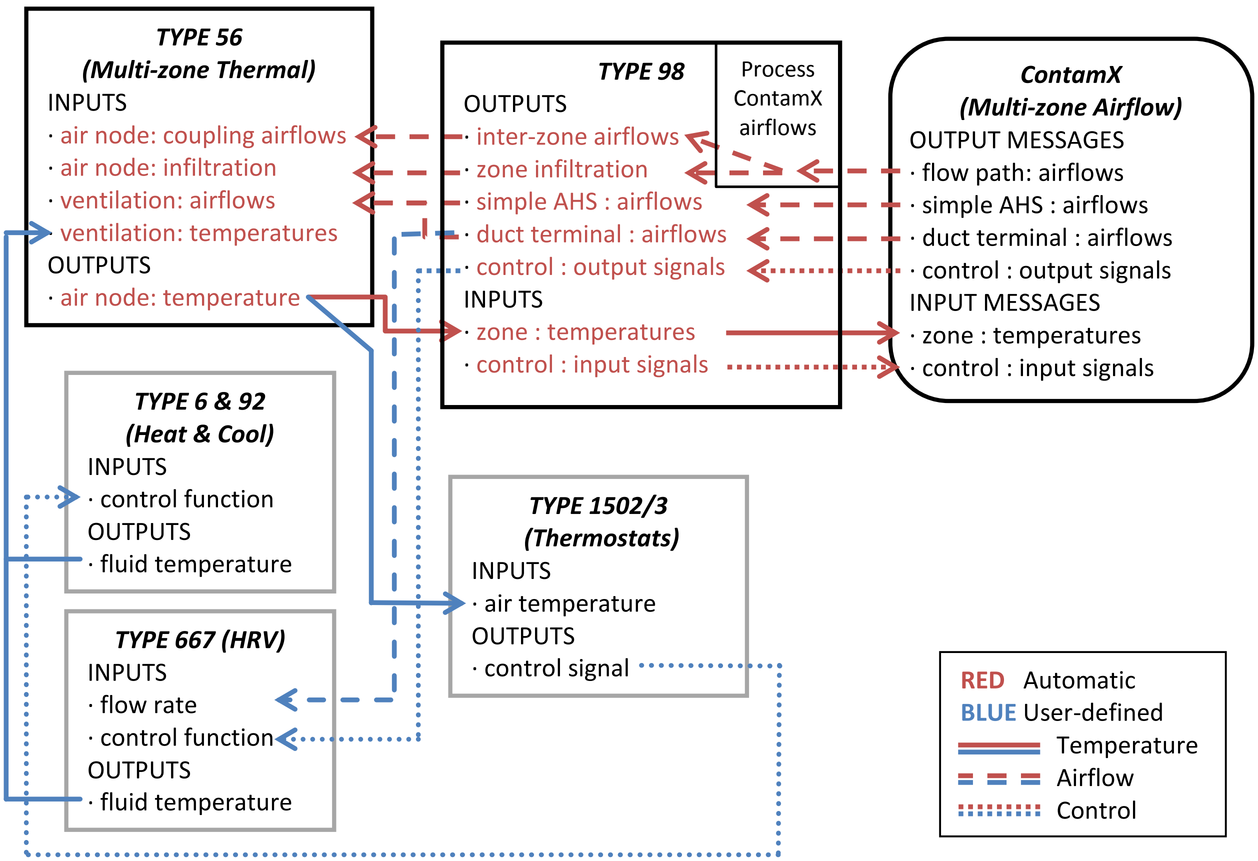


Figure 3. Schematic of TRNSYS Inputs, Outputs and Data Exchange

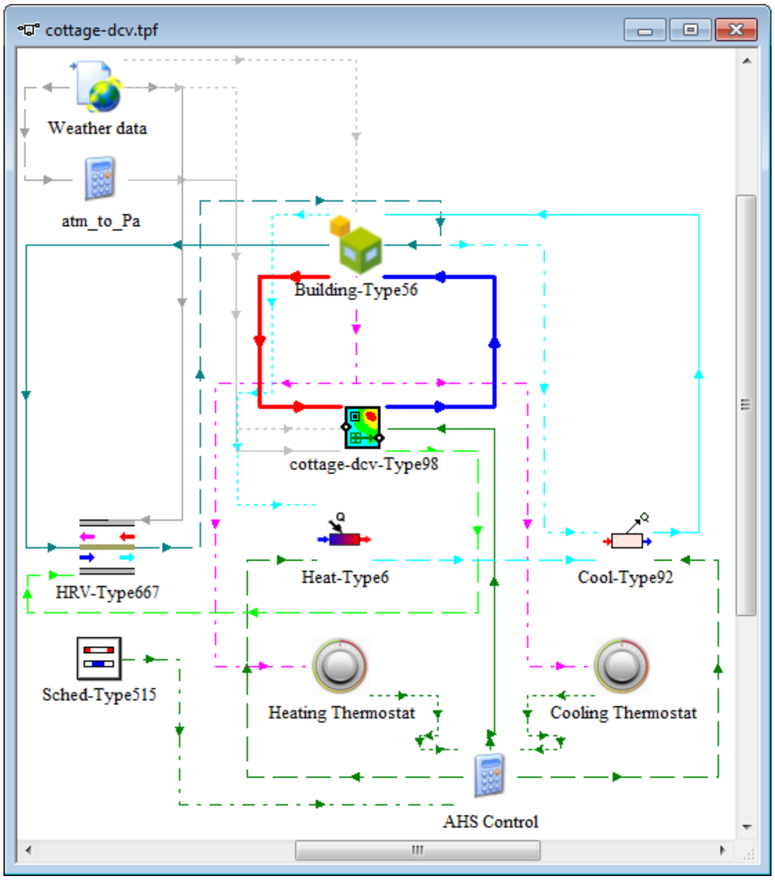


Figure 4. TRNSYS Simulation Studio small house project

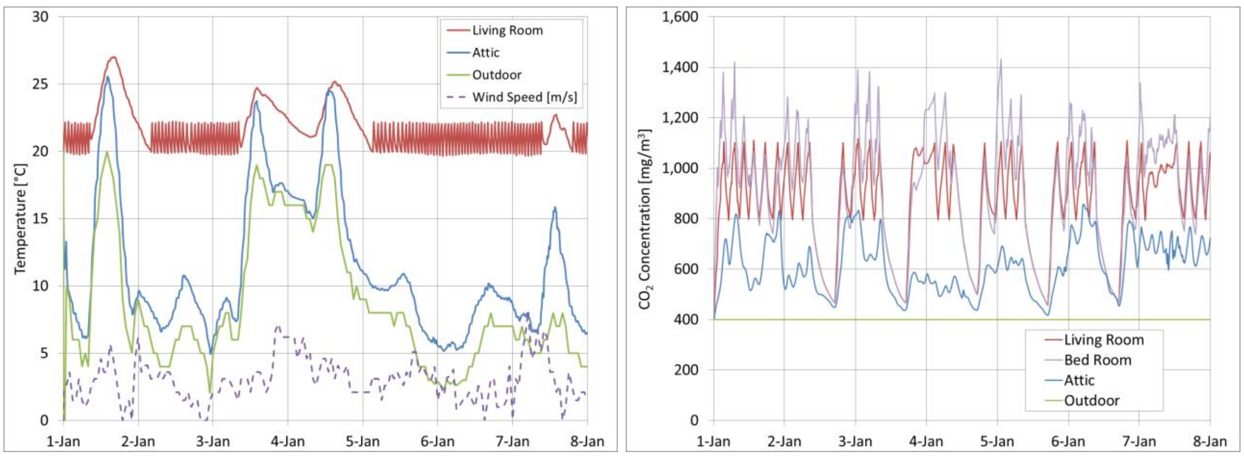
Inter-zone airflows and outdoor airflows into each zone are provided by ContamX to Type 98 which then passes them to Type 56 as *coupling airflows* and *infiltration* inputs, respectively, of Type 56 *airnodes*. CONTAM airflows of the simple air handler and duct system supply air terminals are output from ContamX to Type 98 which passes them to Type 56 as *airnode ventilation* flows.

Zone temperatures are output by Type 56 to Type 98 which passes them to ContamX. The heating/cooling (Type 6 and Type 92) and HRV (Type 667) systems provide temperatures for ventilation flows of Type 56 *airnodes*. Note that temperatures of system flows, i.e., air handling system and duct system supply terminals, are not provided to CONTAM. These temperatures are not significant to CONTAM when the systems are operating. CONTAM duct system temperatures are set by Type 98 to be the same as those of the zones in which they are located. In this manner, if the system fans are not operating, then buoyancy-driven flows will be determined using these temperatures.

The new coupling method provides for the ability to exchange control information with ContamX via Type 98. In this illustrative case, TRNSYS thermostat Types 1502 and 1503 are used to activate the supply flows in both Type 56 and CONTAM. The thermostats provide an on/off control signal that is distributed within the CONTAM model to the air handler supply flows at every time step. The HRV system flows are controlled within CONTAM via a CO_2 sensor located in the central zone of the building. Control logic within the CONTAM model turns the HRV fans in the CONTAM model on or off, and the resultant control signal is passed to TRNSYS via Type 98 and used to activate or deactivate the HRV Type 667 system.

The overall simulation is activated and controlled by TRNSYS. Type 98 establishes communication between TRNSYS and ContamX (which is launched in the so-called bridge communication mode that provides for external communication with ContamX), opens the associated CONTAM project file, and begins transient simulation. Simulation control must be established between CONTAM and TRNSYS in the form of common start/end date/time and calculation time steps.

The results provided below are not meant for model validation purposes but to illustrate the ability to evaluate the interaction between the coupled domains. As shown in Figure 5, coupled simulation enables consideration of the interaction between thermal, airflow and contaminant realms. These plots show indoor temperature fluctuations due to cycling of the heating system in response to temperature (Figure 5a) and fluctuations in CO_2 concentration in response to DCV system (Figure 5b). The simulation time step for this case was three minutes and the thermostat heating setpoint was 21 °C with a deadband of 2 °C (± 1 °C about the setpoint).



(a) (b)

Figure 5. Simulation results exported from CONTAM: (a) indoor and outdoor temperatures and wind speed, and (b) CO_2 concentration

3. Verification test case

A model verification study was performed by comparing simulation results to an analytical solution for a single-zone model with stack-driven ventilation (Yam, Li, and Zheng 2003). The purpose of this verification test case is to demonstrate that the coupling of these two solvers is performing as designed and that the data is being exchanged properly between them.

Figure 6 depicts the building model with two openings at different elevations, an internal heat source, and an extremely large thermal mass. The outdoor temperature varies periodically as a sinusoidal wave, so the stack-driven airflow rate through the building fluctuates accordingly.

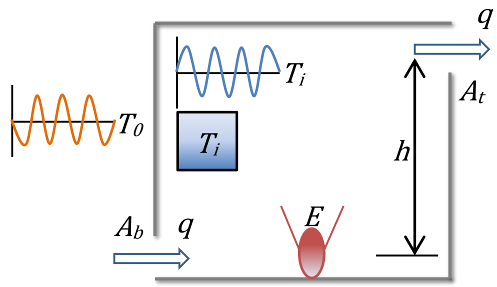


Figure 6. A one-zone building model with two openings, periodic outdoor air temperature variation (T_o), heat source (E), and thermal mass (shaded area) in equilibrium with the room air temperature (T_i)

The energy balance equation for the thermal mass and the associated analytical solution for the volumetric flow rate are provided in equations (1) and (2), respectively. Indoor temperature varies according to equation (3) as influenced by the outdoor temperature which varies according to equation (4).

$$\omega M C_M \frac{\partial T_i}{\partial(\omega t)} + \rho C_p |q|(T_i - T_o) = E \tag{1}$$

$$|q|q = -\frac{2\alpha^3}{\theta} sin(\omega t) + C \tag{2}$$

$$T_i(\omega t) = \left[1 + \frac{C}{2gh(C_d A^*)^2}\right] \tilde{T}_o \tag{3}$$

$$T_o = \tilde{T}_o + \Delta\tilde{T}_o \sin(\omega t) = 300 + 8\, sin\left(\frac{2\pi}{24} t\right) \tag{4}$$

where:

- q = volumetric airflow rate, m^3/s
- T_i = indoor air temperature, °C
- T_o = outdoor air temperature, °C
- $\tilde{T}_o$ = mean outdoor temperature, °C
- $\Delta\tilde{T}_o$ = amplitude of outdoor temperature fluctuation, °C
- ω = frequency of outdoor temperature fluctuation, h^{-1}
- M = mass of large thermal mass, kg
- C_M = heat capacity of thermal mass, J/kg·°C
- C_p = heat capacity of air, J/kg·°C
- ρ = air density, kg/m^3
- α = buoyancy air change parameter, m^3/s
- θ = outdoor temperature fluctuation air change parameter, m^3/s
- t = time, h
- g = acceleration of gravity, m/s^2
- h = distance between two openings, m
- C_d = discharge coefficient
- A^* = effective opening area, m^2

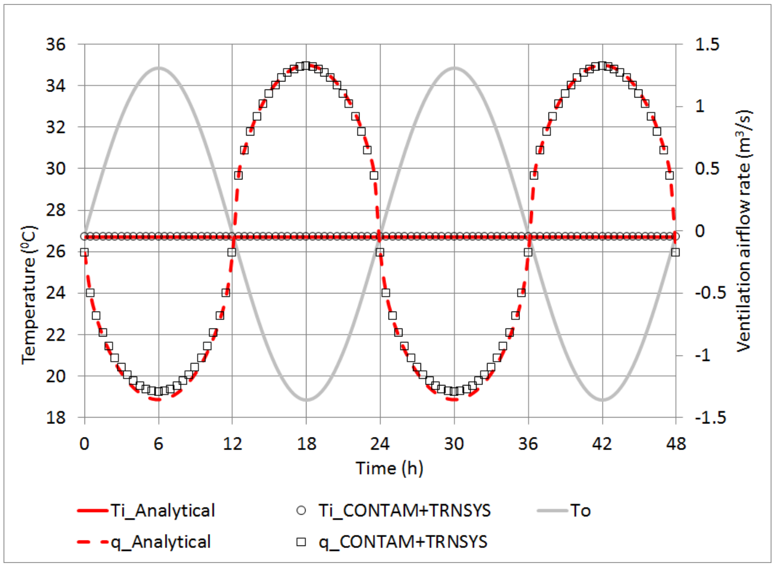


Figure 7. Comparison of coupled simulation results of the airflow rate, q, and the indoor temperature, T_i, with the analytical solution (Note that not all points are shown for the simulated results)

Figure 7 shows that the stack-driven flow varies at the same 24-hour cycle as that of the outdoor temperature. The thermal mass is extremely large so the indoor temperature is almost constant even with a heat source. When the temperature difference, $T_o - T_i$, reaches a maximum, the flow rate, q, also reaches an out-of-phase maximum as shown in Figure 7. The coupled simulation provides nearly identical results as the analytical solution providing verification of the coupled thermal/airflow calculations. Note that very minor differences in flow rate occur at the highest and lowest temperatures, because it was not possible to use an infinitely large mass in the simulation.

The ability to successfully obtain the proper solution to this problem does not indicate that this coupling can address all possible combined heat transfer and airflow problems. In fact, Li, et al., have shown that for a certain class of problems the coupling of the heat transfer and airflow regimes suffer from potential multiple solutions (Li et al. 2001). Specifically, multizone models addressing natural ventilation under conditions of opposing wind and thermal buoyancy forces could experience solution stability issues. While the basis of this observation was the analysis of a simple two-zone building and scale model, Axley, et al. revealed such numerical instabilities in a previous coupled model demonstration on a naturally ventilated, three-storey office building (Axley, Emmerich, and Walton 2002). This is an area of future research required to address the ramifications of multiple solutions, limitations of the quasi-dynamic coupling approach as well as the uncertainty involved in implementing this quasi-dynamic co-simulation technique.

4. Application – impact of vestibules on building energy consumption

According to the *Buildings Energy Databook* (Table 1.1.4 in (DOE 2012)), the U.S. consumed 19 % of the global energy in 2010, and the building sector (residential, commercial and government) accounted for about 41 % of the primary U.S. energy usage. The top four end uses of the building sector are space heating (37 %), space cooling (10 %), water heating (12 %), and lighting (9 %), for a total of about 70 % of building site energy consumption. Table 1 illustrates the relative components of heating and cooling loads for commercial buildings based on computer simulations of 120 commercial building prototypes (Huang and Franconi 1999). 18 % of the total heat loss was due to air infiltration. The results in Table 1 are based on a study that utilized DOE-2, and the method of estimating infiltration is not provided in the documentation of these studies. Doorway airflows can be a significant component of infiltration when doors are used more frequently as in restaurants, retail stores, supermarkets, offices and hospitals. Reducing these airflows may represent significant potential savings in whole building energy usage. The updated coupling approach provides for addressing individual components of infiltration, and the following application of the updated coupling approach addresses the issue of energy loads attributed to doorway airflows.

Table 1. Aggregate commercial building component loads as of 1998 (Table 3.1.12 in (DOE 2012))

Component of Net Load	Heating [% of Net]	Cooling [% of Net]
Roof, Walls, Foundation	12, 21, 11	1, -, -
Infiltration	18	-
Ventilation	15	-
Windows – conduction, solar	22, -	-, 32
Lights	-	42
Equipment – electrical, non-electrical	-	17, 1
People	-	7

ASHRAE Standard 90.1 (ANSI/ASHRAE/IESNA 2010) requires vestibules in climate zones 3 – 8 in order to reduce air infiltration through entrance doors. The Pacific Northwest National Laboratory (PNNL) (Cho, Liu, and Gowri 2010) conducted a series of energy modeling studies using EnergyPlus that found vestibules can achieve energy savings of up to 5.6 % for the prototype buildings that were modeled. Moreover, the energy saving potential could be even higher for the buildings with frequent door usage, e.g., strip malls, standalone retail, and fast-food restaurants. PNNL estimated the volumetric airflow rate through vestibules based on the empirical model developed by Yuill (Yuill 1996; Yuill, Upham, and Hui 2000) shown in equation (5).

$$Q = C_A A R_P \tag{5}$$

Q = airflow through doorway, m^3/s
C_A = airflow coefficient, $m^3/s{\cdot}m^2{\cdot}Pa^{0.5}$
A = area of door opening, m^2
R_P = pressure factor, $Pa^{0.5}$

C_A and R_p were determined by Yuill based on three assumptions: (1) wind speed of 6.7 m/s, (2) neutral pressure plane located at mid-height of the building, and (3) a thermal draft coefficient of 0.9 indicating internal resistance to airflow slightly reduces the stack effect pressure from the theoretical maximum. Correlations were developed by Yuill for C_A as a function of door-opening frequency and for R_P as a function of building height and outdoor air temperature. Using these correlations, air infiltration through entry doors was calculated for a constant outdoor air temperature of 15.6 °C. PNNL also performed a sensitivity study over a range of door opening frequencies and outdoor temperatures between -40 °C and 26.7 °C that revealed peak infiltration rates were more dependent on door opening frequency than outdoor temperature.

In reality, outdoor temperature, wind speed and direction can vary significantly over time. The door flow rate of equation (5) is based on the assumption that the pressure factor remains constant. Yuill (Yuill 1996; Yuill, Upham, and Hui 2000) pointed out that it is a rough estimation of doorway flows, and suggested that a better approach would be to use multizone airflow modeling to estimate the changing pressure difference. In order to better account for the variation in pressure difference across the building entrance, the new coupled TRNSYS/CONTAM model is applied to study the impact of various building entryway configurations on whole building energy use.

4.1 Case Description

This study focuses on a three-story medium office building (Deru et al. 2011), which is one of the building models used in the PNNL study and is depicted in Figure 8. Two different entryway configurations were implemented: a single set of double swinging doors and a vestibule with double swinging doors. NIST developed CONTAM models of this office building, along with the whole set of DOE reference commercial buildings (Ng et al. 2012). In order to properly model the building airflow, the CONTAM model was slightly modified from the original thermal zoning of the EnergyPlus models to include both stair and elevator shafts that span all four floors of the building and a restroom on each floor as shown in Figure 8 through Figure 10. The entry door was simulated to operate between 7:00 and 19:00 Monday through Saturday and to be closed all day Sunday. Annual simulations were performed with Chicago weather conditions and four different building orientations.

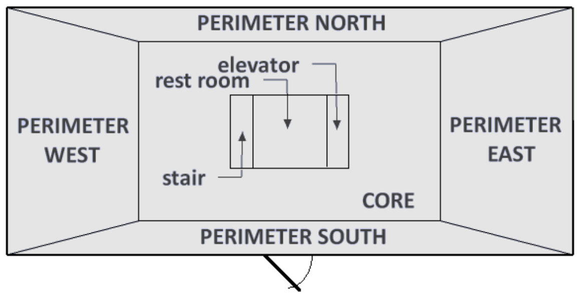


Figure 8. Floor plan of medium office building

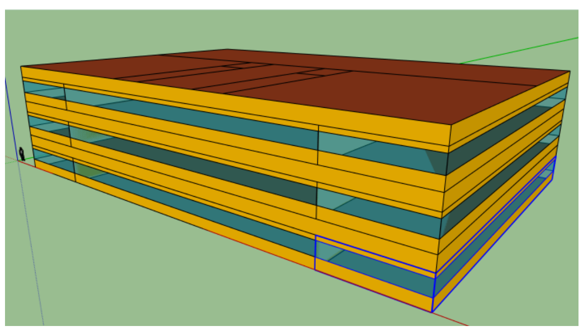


Figure 9. Trnsys3d representation of medium office building

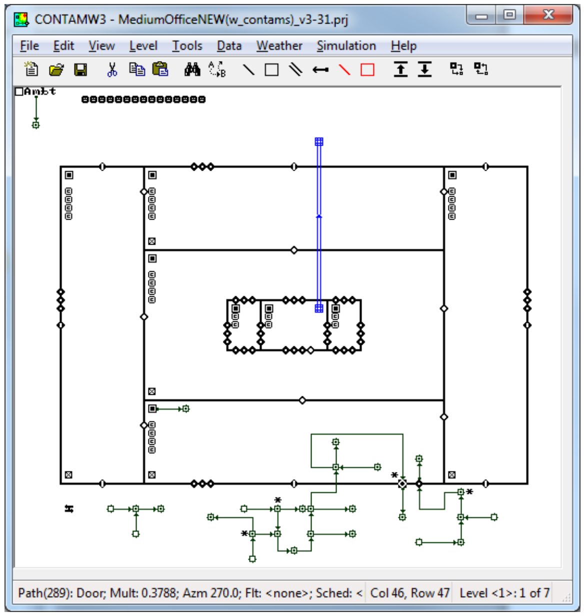


Figure 10. CONTAM model of medium office building

Yuill (Yuill 1996; Yuill, Upham, and Hui 2000) conducted experiments using scale models to determine average discharge coefficients for the orifice equation for building entrances with and without vestibules. These coefficients accounted for door usage frequency, geometry, and pressure difference across the doorway. It was found that vestibule doors lead to smaller discharge coefficients and thus lower infiltration than entranceways having no vestibule. The time-averaged discharge coefficients, C_{Dave}, based on Yuill's experiments (see Table D-1.9 in (Yuill 1996)) were converted to a flow coefficient, C, for a 4.8 m^2 door area. These values are listed in Table 2.

Table 2. Flow coefficients for building entrances based on a usage frequency of 100 people/hour

Entrance Type	Person Per Usage	Door Usage per hour	Average Discharge Coefficient C_{Dave} (-)	Flow Coefficient C (m^3/s·Pa$^{0.5}$)
Single door	2.7	37	0.4625	0.5554
Vestibule door			0.3666	0.3788

4.2 *Results and Discussion*

Figure 11 presents hourly predictions of pressure difference across the entrance, airflow through the entrance and indoor (Perimeter South zone) temperature for the case when the vestibule entrance is facing the dominant wind direction. The pressure difference across the vestibule door ranges from -10 Pa to 45 Pa but is typically between -10 Pa and 10 Pa. The resultant volumetric flow rate through the vestibule door ranges from -1 m^3/s (flow to outdoors, outflow) to 2.2 m^3/s (flow from outdoors, inflow). The winter season is dominated by inflow through the doorway causing significant heating loads, whereas outflows dominate in the summer. Another factor affecting the energy impact of the vestibule door is the indoor and ambient temperature difference as shown in Figure 11(c). The indoor temperature is well controlled within 15.6 °C and 26.7 °C (including night and weekend setback) by the HVAC system as the ambient temperature varies from -23 °C to 35 °C over a year.

Table 3 provides a comparison of the annual average inflow and outflow rates between the vestibule door and the single door for different door-facing directions. The door facing the west (predominant wind direction) will cause the highest average inflow of 0.73 m^3/s for the single door and 0.56 m^3/s for the vestibule door. The corresponding reduction of inflow using the vestibule relative to the single door is around 23 %. For other door directions, the reduction of inflow by the vestibule is about the same. The reduction of outflow for different door directions is also about 25 %.

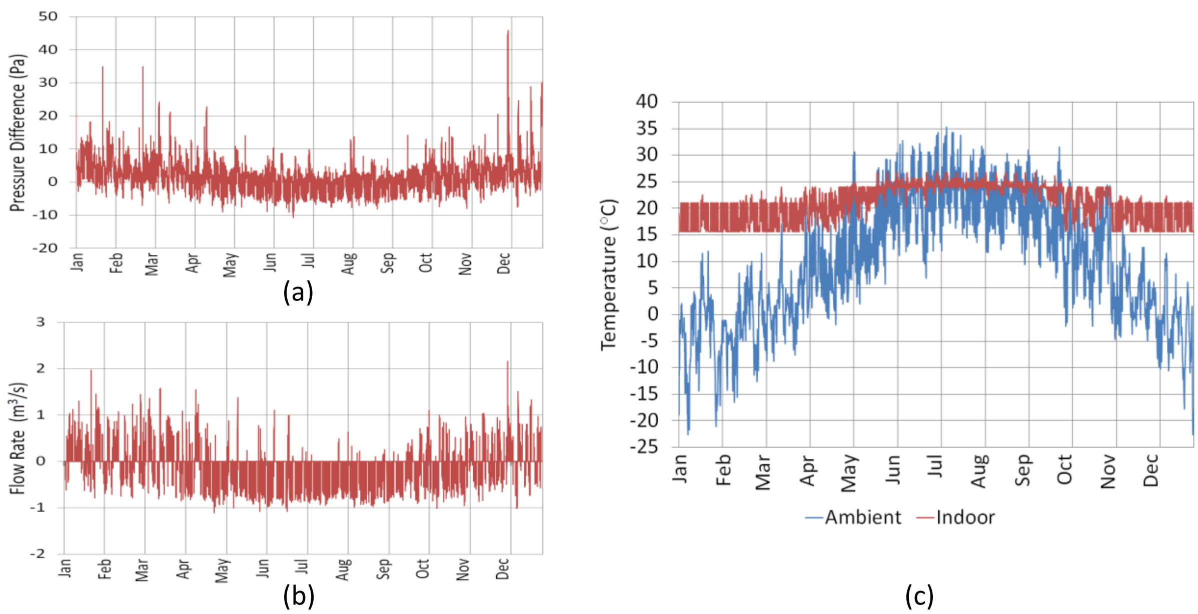


Figure 11. The predicted (a) pressure difference and (b) flow rate through the vestibule door, and (c) indoor temperature for vestibule entrance facing the predominant wind direction

Table 3. Annual average airflow rates and reduction for vestibule door compared to single door

		East	South	West	North
Average rate of inflow through the doorway (m^3/s)	Single Door	0.45	0.61	0.73	0.69
	Vestibule Door	0.37	0.47	0.56	0.53
Average rate of outflow through the doorway (m^3/s)	Single Door	0.77	0.75	0.77	0.80
	Vestibule Door	0.58	0.56	0.58	0.60
Annual reduction of inflow due to vestibule (%)		22	23	23	23
Annual reduction of outflow due to vestibule (%)		25	25	25	25

From the airflow through the doorways and the indoor and outdoor temperatures, an estimate of the time-dependent energy demand due to inflow through the door is obtained by the following equation.

$$E_{door} = \rho Q_{door} C_p |T_i - T_o| \quad (6)$$

where:

E_{door} = energy demand due to airflow in through the door, kW
ρ = air density, kg/m^3
Q_{door} = volumetric airflow rate (≥ 0) through the door, m^3/s
C_p = specific heat of air, 1.005 kJ/kg·˚C
T_i = indoor air temperature of the entry zone, ˚C
T_o = ambient air temperature, ˚C.

Based on equation (6), the transient energy loss due to infiltration through the doorway can be calculated and comparisons made between the single door and vestibule as shown in Figure 12. The largest savings come from the door facing west and north, especially during the winter seasons. The energy demand savings over a 30 minute period can be as high as 30 kW for the door facing north. During the summer seasons, outflow occurs most of the time, and the effect of the vestibule is limited due to the relatively small inside/outside temperature difference. Therefore, most savings attributed to the vestibule occur during the heating season.

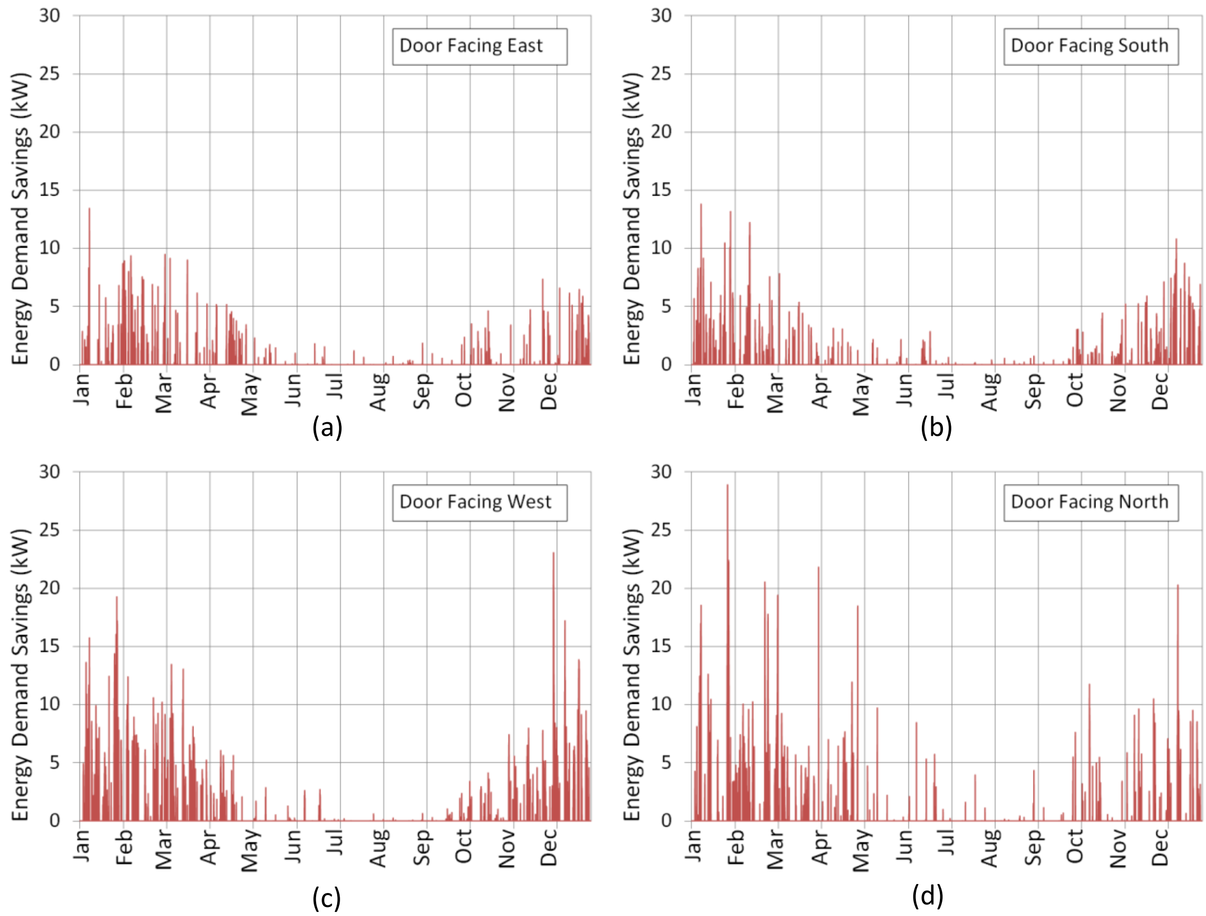


Figure 12. The reduction of the energy loss due to doorway flow by using the vestibule door when compared to the single door for the DOE medium office in Chicago when the door faces (a) east, (b) south, (c) west and (d) north (plotted every 30 minutes)

Figure 13 shows the annual total heating and cooling loads when the vestibule door is used compared to the single door. It was found that the whole building energy saving of the vestibule can reach 3.7 MWh for the door facing west, which is a saving of 1.4 %. The average energy savings over all four building orientations is about 2.7 MWh (1.0 %). The annual cooling load slightly increases for the vestibule case, because the vestibule reduces the amount of free cooling that occurs during the shoulder seasons in the single door case.

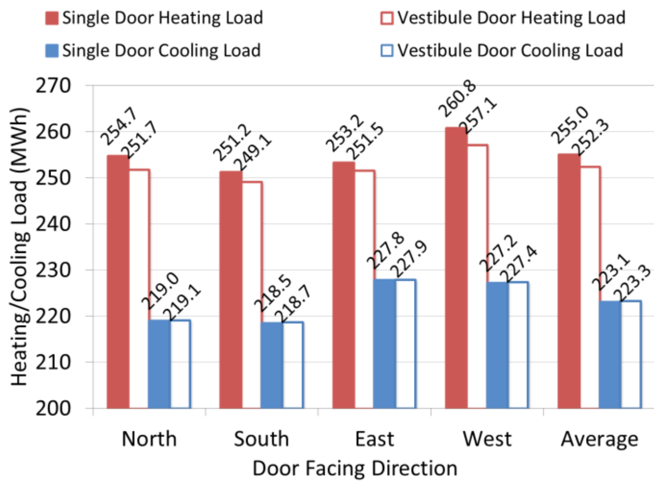


Figure 13. The annual total heating/cooling energy use of the vestibule door when compared to the single door for the DOE medium office at Chicago for different door facing directions

In summary, by using the coupled TRNSYS and CONTAM simulations, we are able to predict annual time-dependent infiltration and exfiltration rates through building entrance doors, their impact on the energy loss through these openings, and the resultant whole building heating and cooling loads. It was found that for the modeled DOE medium office building, the use of the vestibule can achieve a reduction in the airflow through the building entry door of 23 % annually. The resultant whole building energy saving can be as high as 1.4 %, which is 3.7 MWh annually, when compared to the building entrance without the vestibule. The average percentage saving over four building orientations is 1.0 % (2.7 MWh), which is higher than the savings of 0.26 % estimated for the medium office building in the PNNL study (Cho, Liu, and Gowri 2010). This difference is likely due to differences in the methods used to determine the doorway flows. The PNNL study used equation (5), which assumes a constant outdoor air temperature and constant wind speed, whereas this study considered transient ambient conditions, i.e. outdoor temperature, wind speed and direction, and their effects on building pressures.

5. Conclusions

The design and analysis of high performance buildings to meet demanding energy and IAQ goals increasingly requires advanced building modeling capabilities to simultaneously model heat transfer, airflow and pollutant transport. An updated multizone building heat transfer, airflow and contaminant transport simulation tool was developed through loose, *quasi-dynamic* coupling of the TRNSYS energy simulation program with the CONTAM multizone airflow and IAQ model. Along with new supplementary utilities, this second generation coupling greatly expands functionality and increases usability of coupled building energy and airflow simulation by adding multizone contaminant transport, adding access to all of the airflow modeling components of CONTAM (including the capability to simulate air handling systems and detailed duct networks), and incorporating automatic formation of temperature and airflow connections between the building energy and airflow models.

Application of the new coupled tool was demonstrated for a simple case of a small house with CO_2-based DCV, an analytical airflow/heat transfer test case, and a practical design problem of airflow through entry doors in non-residential buildings. It was found that for the modeled medium office building, the use of the vestibule can reduce infiltration through a building entrance by 23 % and can save 1.4 % of the whole building heating and cooling energy use annually, when compared to the building entrance without a vestibule.

Coupling Limitations and Future Work

The implementation presented herein, was an initial step in coupling the whole-building energy simulation capabilities of TRNSYS Type 56 directly with the CONTAM airflow and contaminant transport simulation engine (ContamX) as opposed to the partial implementation of CONTAM performed via TRNSYS Type 97. As such, there is more work to be done in order to provide more complete coverage of capabilities provided within the coupled tools and to establish the ability of the coupled tools to accurately address various modeling applications.

Dynamic vs. Quasi-dynamic Coupling

This coupling between the heat transfer and airflow domains was performed using the quasi-dynamic method. This method, while simpler to implement, requires the use of relatively short time steps in order to maintain accuracy but may lead to increased simulation times. Investigation of implementing the dynamic coupling method is warranted, but there are inherent difficulties related to this method in the form of applying stability control, e.g., relaxation coefficients, between the segregated simulation environments. Work needs to be done to investigate the limitations and accuracy of the current coupling method and the potential implementation of the dynamic method.

Simulation Initialization

The current coupling method does not provide the ability to perform coordinated *warm-up* simulations. This so-called warm-up period enables the loading of thermal and contaminant storage capacities (e.g., thermal mass and contaminant sorption) in the energy and contaminant transport models, respectively. As such, simulations require that an initial time period be allotted for this capacitance-loading to occur. In order to overcome this limitation, it is likely that Type 56, ContamX and Type 98 would require modification.

Moisture Transport

Accounting for moisture transport is important to many aspects of building performance including energy (latent heat loads), IAQ (mold growth and effects on contaminant transport properties, e.g., absorption rate) and life expectancy of building materials. The coupling process implemented as described within this paper does not account for the coupling of moisture between the energy and airflow/contaminant transport simulation tools. This should be a target of future development.

CFD

As briefly presented in the Introduction, CONTAM is capable of using CFD to simulate the detailed airflow and contaminant transport field of a single zone within a multizone model. However, this capability is not currently available via the coupling method presented in this paper. This capability would lend itself well to the consideration of large zones such as atriums and conference rooms.

Empirical/Experimental Validation

While this paper presented a relatively simple verification test case, it did not include any empirical or experimental validation cases. Although, both tools have been applied in multiple design and analysis projects, it is important to address the applicability of the coupled method to cases that are expected to be readily addressable as well as those that would be expected to challenge the coupled solution method. The former being considered regression test cases (i.e., the coupling does not cause the existing implementations to regress and perform worse than the uncoupled approaches) based on buildings that implement more traditional mechanical heating, ventilating and air-conditioning systems, and the latter including the more challenging natural ventilation cases where-in opposing wind and buoyancy forces come into play.

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