Project Title: An Indoor Environment Design Tool for Entire Buildings

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1. Specific Aims

The main project aim was to develop an integrated design tool to analyze combined problems of Indoor Air Quality (IAQ) and thermal comfort for an entire building. The original aim has not been changed. The main success of the project is that the integrated tool is developed and that it was used for several cases studies. The tool was validated with on site-data, a step that no other study in this area has ever performed before. Further improvements of the integrated tool should be made to sustain the project's long term vision of having this technology readily available in building design industry.

2. Studies and Results

The developed integrated tool has three major components: (1) building heat transfer and fluid flow models, (2) a heating, ventilating, and air-conditioning (HVAC) model, and (3) mass and heat source/sink models. The building models use a simplified CFD model to calculate IAQ and thermal comfort in a single zone and a multi-zone model, CONTAMW, to link the heat and mass transfer between zones for an entire building. The HVAC model use modules that can be easily used to form different HVAC systems. The mass and heat source/sink models use the coupled program of the modified CONTAMW and an energy analysis program, EnergyPlus, as well as various dispersion models. Therefore, the new integrated tool uses:

- the modified multi-zone model CONTAMW
- the simplified computational fluid dynamics program CFD0
- the energy analysis program EnergyPlus.

All of the programs are intergraded through coupling procedures to enhance performance of each individual program in IAQ and thermal comfort calculations for an entire building.

2.1 Coupling of Multi-Zone and Energy Programs

Multi-zone models are widely used to predict the contaminant distribution within whole buildings. However, typically multi-zone models do not incorporate energy equations to consider building heat transfer. An ordinary practice is to assume an isothermal condition or assign a pre-described temperature profile for the simulated zones. However, this practice is a challenging task even for experienced users, because guessing a correct temperature distribution is difficult and multi-zone simulations are sensitive to the temperature distribution. This project demonstrated the multi-zone sensitivity to temperature distribution and clearly showed that a temperature guessing error of only 2°C can cause not only wrong air and contaminant flow rates but also a wrong direction for the flow rates. These kinds of calculation errors result in completely wrong contaminant distribution in a building. Therefore, an algorithm is developed to introduce energy load calculations into a multi-zone model. The study provides temperature prediction by combining the airflow modeling from a multi-zone program and the load calculation from an energy program. The combined model predicts the indoor contaminant distribution with calculated temperature distribution and in this way increases the accuracy of IAQ predictions by correct calculations of contaminant distribution.

The new enhanced multi-zone method was applied to a cubicle floor in an office building for a 24-hour dynamic simulation. A full-scale transient Computational Fluid Dynamics (CFD) simulation was also conducted for the validation of contaminant distribution results obtained from a multi-zone model. The results show that the enhanced multi-zone-energy method provides better prediction of contaminant distribution than the multi-zone model alone, especially in variable thermal loads with variable air volume HVAC system. In addition, the combined method demands much less computational time than CFD method. The calculation time savings of the multi-zone model compared to CFD is particularly evident for dynamics simulation cases. When appropriately applied in building simulations, the combined multi-zone-energy simulation method can accurately predict contaminant distribution without prior knowledge of temperature distribution.

2.2 Coupling of CFD and Multi-Zone Programs

The project also worked on improvements of multi-zone models for predicting building contaminant distribution by combining a multi-zone model with a Computational Fluid Dynamic (CFD) model. The motivation was to avoid the long computations and long model input in the CFD program that are required for predicting concentrations in entire buildings. Two cases are investigated using the combined model and the results are compared to reliable experimental or CFD data. The primary purpose of the two studied cases was to explore the feasibility and effectiveness of the combined method. Heavily partitioned offices instead of a whole building were selected for our project because reliable experimental data for Case 1 existed, and we conducted measurements for Case 2. The study results indicate that the combined model should be used only when a non-uniform distribution of contaminants is expected such as in Case 2. Furthermore, the simulations demonstrated time-saving benefit of the combined method. It is very expensive to conduct CFD simulations to predict contaminant concentrations in an entire building, especially for the building conceptual design when many different design solutions should be tested. In this kind of situation, combined multi-zone and CFD models become necessary.

Our findings in the simulated two cases are useful for defining and fine-tuning similar simulations in the future. The best methodology for coupling the two models becomes an important question to consider. For example, an iterative procedure for boundary conditions exchange between CFD and multi-zone models might be required.

2.3 New Contaminant Source/Sink Models

Recent studies have shown that elevated indoor concentrations of volatile organic compounds (VOCs) emitted from building materials can have adverse effects on indoor air quality and human health. The integrated design tool can be used for indoor air quality and ventilation analyses because it calculates airflow, contaminant concentration and personal exposure in a building. However, the currently available contamination source/sink models in CONTAMW do not include recently developed VOC source/sink models for new building materials.

List of Incorporated VOC Source/Sink Models

Models		Parameters	Determination of model parameters
Emission models	Internal diffusion-controlled emission model	k, F0	Direct measurement
	Double exponential equation	a, b, k1, k2	Curve fitting
	Exponential-power equation	a, b, c, d, f	Curve fitting
	Diffusion-controlled emission model	C_0, K, D	Direct measurement
Sorption models	Numerical sorption model	K, D	Direct measurement

Five new source/sink models are successfully incorporated and tested in CONTAMW to enable studies on VOC dispersion in buildings. The incorporated models are: two diffusion controlled emission models, double exponential model, exponential power model and numerical sorption model. Furthermore, an on-site experiment has been conducted to demonstrate the applicability of a VOC source model to a real building. The experiment used SF_6 to validate prediction of airflow rates, with measurements for total volatile organic compounds (TVOC). The calculated and measured data agree well with a few local larger discrepancies. This result is encouraging because it shows that the model can be applied in real buildings.

With these new models, it will be possible to predict the indoor VOCs concentration resulting from building material with known emission/adsorption properties such as certain types of carpets, paints or linoleum. The simulation results can be used to prevent or mitigate poor indoor air quality with better design of ventilation and better selection of construction materials.

2.4 Strengths and Weaknesses the Current Integrated Tool

The main strengths of the new integrated design tool is its capabilities to simulated complicated indoor air quality and thermal conditions for an entire building very quickly within a couple of seconds to a couple of hours depending on the complexity of the problem. Additional strength of this integrated program is that we conducted validation in a real building. Figure 1 shows the layout and instrumentation in one of the two different locations that we used to conduct the measurements. The experiments were limited to one highly partition space due to the extreme labor and time needed to collect such high quality data.

This technology is completely new, and, therefore, needs additional developments to enter standard design practice. Our project revealed the following areas to be the most important for further dissemination of this technology:

(1) interface
(2) coupling methods

(3) criteria for using the program components
(4) additional case studies

An interface would help to dissemina6e this technology to much larger audience than the audience willing to learn about each of the components of the integrated program. There are many additional issues and methods to optimize and improve the coupling between the components of the integrated program. In addition, a clear mathematical condition or conditions would help select which program components to use for a particular case. Finally, additional case studies would serve as an excellent training ground for new users. The participants in this project will seek additional funding to further develop this powerful technology.

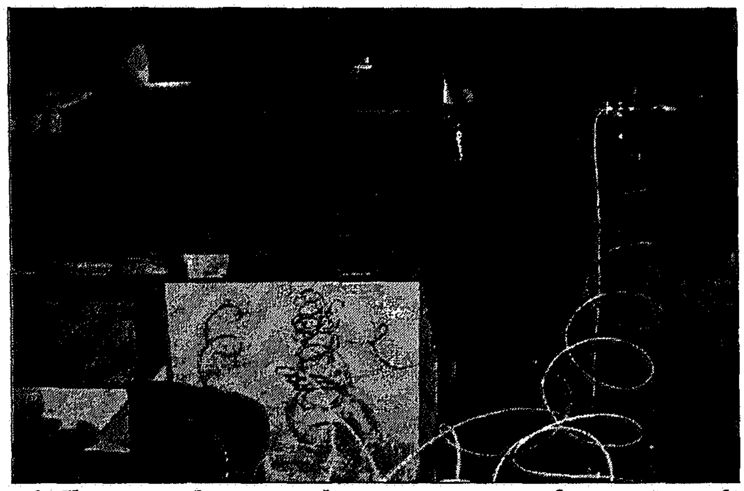

Figure 1 The space layout and instrumentation for on-site validation

3. Significance

The significance of the current findings is that an accurate prediction of indoor contaminant distribution is possible to be performed quickly on a desktop PC. Ultimately, these predictions will unable quick and accurate stüdies on contaminant exposure for different individuals in different parts of a building.

4. Publications

Published papers and thesis:

Hu, H. and Srebric, J. 2004. "Indoor VOC source and sink modeling in multizone simulations of real buildings," CIB World Building Congress 2004, CD ROM, paper no. 820, 11 pages, Toronto, Canada.

Yuan, J. and Srebric, J. 2004. "Transient prediction of contaminant distribution by introducing energy load calculations into multi-zone modeling," CIB World Building Congress 2004, CD ROM, paper no. 148, 11 pages, Toronto, Canada.

Yuan, J. 2003. "Effective Prediction of Air Distribution and Contaminant Transport in Entire Buildings by Coupling Multi-Zone, CFD and Energy Models," M.Sc. Thesis, Dept. of Architectural Engineering, The Pennsylvania State University, August 2003, 80 pages.

Yuan, J. and Srebric, J. 2002. "Improved prediction of indoor contaminant distribution for entire buildings," American Society of Mechanical Engineers (ASME), Fluids Engineering Division (Publication) FED, v 258, 2002, p 111-118.

Publications under preparation:

Srebric, J., Yuan, J., and Novoselac A. 2005 "On-Site Experimental Validation of a Coupled Multi-zone and CFD model," for Int. J. of Ventilation.

Yuan, J. and Srebric, J. 2005. "Multizone modeling in real buildings with transient heat transfer and non-uniform contaminant distribution," for Building and Environment.

5. Project-Generated Resources

The current version the integrated software can be obtained by contacting the PI:

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FINANCIAL STATUS REPORT

(Short Form)

1. Federal Agency and Organizational Element to Which Report is Submitted	2. Federal Grant or Other Identifying Number Assigned by Federal Agency	OMB Approval No.	Page	of
DHHS - Center for Disease Control	5 K01 OH007445-03	0348-0039	1	1 pages

The Pennsylvania State University
Research Accounting
313 Rider Building
120 S. Burrowes Street
University Park, PA 16801

4. Employer Identification No.	5. Recipient Account Number or Identifying Number	6. Final Report	7. Basis
124-6000-376	415-17 NIH DESIGN TOOL 200 (51NA)	[X] Yes [ ] No	[x] Cash [ ] Accrual

8. Funding/Grant Period From: (Month, Day, Year)	TO: (Month, Day, Year)	9. Period Covered by this Report From: (Month, Day, Year)	TO: (Month, Day, Year)
08/01/2001	07/31/2004	08/01/2003	07/31/2004

10. Transactions:	I Previously Reported	II This Period	III Cumulative
a. Total outlays	95,843.56	64,235.44	160,079.00
b. Recipient share of outlays	0.00	0.00	0.00
c. Federal share of outlays	95,843.56	64,235.44	160,079.00
d. Total unliquidated obligations	[redacted]		0.00
e. Recipient share of unliquidated obligations			0.00
f. Federal share of unliquidated obligations			0.00
g. Total Federal share (Sum of lines c and f)			160,079.00
h. Total Federal funds authorized for this funding period			160,079.00
i. Unobligated balance of Federal funds (Line h minus line			0.00

11. Indirect Expense	a. Type of Rate	[ ] Provisional	[X] Predetermined	[X] Final	[ ] Fixed
	b. Rate 8.00 %	c. Base $49,168.52	d. Total Amount $3,933.44	e. Federal Share $3,933.44	

12. *Remarks: Attach any explanations deemed necessary or information required by Federal sponsoring agency in compliance with governing legislation*

13. Certification: I certify to the best of my knowledge and belief that this report is correct and complete and that all outlays and unliquidated obligations are for the purposes set forth in the award documents.

Typed or Printed Name and Title	Telephone (Area Code, number and extension)
Michelle L. Bonsell Supervisor-Research Accounting	(814)865-7525
Signature of Authorized Certifying Official	**Date Report Submitted**
[signature]	09/22/04

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OMB No. 0925-0001

Department of Health and Human Services

Final Invention Statement and Certification

(For Grant or Award)

DHHS Grant or Award No.

K01 OH007445

A. We hereby certify that, to the best of our knowledge and belief, all inventions are listed below which were conceived and/or first actually reduced to practice during the course of work under the above-referenced DHHS grant or award for the period

08/01/2001 through 07/31/2004.

original effective date — *date of termination*

B. Inventions (Note: If no inventions have been made under the grant or award, insert the word *"NONE"* under Title below.)

NAME OF INVENTOR	TITLE OF INVENTION	DATE REPORTED TO DHHS
Jelena Srebric	NONE	
(Use continuation sheet if necessary)		

C. First Signature —The person responsible for the grant or award is required to sign (in ink). Sign in the block opposite the applicable type of grant or award.

TYPE OF GRANT OR AWARD	WHO MUST SIGN *(title)*	SIGNATURE
Research Grant	Principal Investigator or Project Director	
Health Services Grant	Director	
Research Career Program Award	Awardee Dr. Jelena Srebric	[signature]
All other types (*specify*):	Responsible Official	

D. Second Signature — This block *must* be signed by an official authorized to sign on behalf of the institution.

Title	Name and Mailing Address of Institution
Associate Vice President for Research	Robert Killoren Office of Sponsored Programs The Penn State University 110 Technology center 200 Innovation Blvd. University Park, PA 16802-7000
Typed Name: Robert Killoren	
Signature: [signature] — Date: 03/03/2005	

HHS 568 (Rev. 9/2004)