2009 BFRL Project Description

Project Title: Advanced Aerosol Transport Modeling for Indoor Environmental Analysis

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BFRL Program: Healthy and Sustainable Buildings

Objective: To advance particle modeling capabilities in support of the design, operation and maintenance of buildings with healthy indoor environments under both normal and adverse circumstances.

Problem:

What is the problem? Particulate contaminants are known to be a health issue with respect to asthma[1], as well as other acute respiratory exposures associated with infectious agents and chemical, biological and radiological (CBR) events. The need to address particle-related health impacts, particularly related to asthma, has been identified as a major indoor air quality issue[2]. In terms of CBR-related applications, several federal agencies are responding to congressional concerns about the adequacy of existing biosampling strategies, and a better understanding of particulate transport and fate is acknowledged as key to addressing these concerns[3]. In addition, concerns are being raised about the potential health risks of engineered as well as ambient nanoparticles, and very little is understood about their transport and associated exposure[4]. Multizone building airflow and contaminant transport models are applicable to a wide variety of indoor environmental challenges including establishing and maintaining healthy indoor environments within buildings subject to day-to-day use as well as extreme conditions resulting

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1 *Clearing the Air: Asthma and Indoor Air Exposures*, Institute of Medicine, Division of Health Promotion and Disease Prevention, National Academy Press, Washington, D.C., (2000).

2 *Research Priorities for Airborne Particulate Matter·IV: Continuing Research Progress*, National Research Council, National Academy Press, Washington, D.C., (2004).

3 *ANTHRAX DETECTION: Agencies Need to Validate Sampling Activities in Order to Increase Confidence in Negative Results*, Report to the Chairman, Subcommittee on National Security, Emerging Threats, and International Relations, House Committee on Government Reform, House of Representatives. GAO-05-251, U.S. Government Accountability Office, Washington, D.C., (2005).

4 The National Nanotechnology Initiative Strategic Plan. Subcommittee on Nanoscale Science, Engineering and Technology, National Science and Technology Council, (2007)

from CBR and fire-related events. However, these models do not currently address the unique mass transport mechanisms associated with particles and other aerosols.

Why is it hard to solve? Particle and aerosol transport modeling requires the consideration of multiple mass transport phenomena that are not currently implemented in multizone modeling tools. Where gaseous pollutants can typically be characterized as ideal gases at trace levels transported primarily through advection and diffusion, particles involve very different transport processes that are a function of particle properties. Among the transport mechanisms that need to be considered are deposition onto internal surfaces, relative humidity impacts, electrostatic forces, agglomeration and coagulation to form larger particles, and resuspension from surfaces. Not all of these transport mechanisms are sufficiently well understood for implementation in building contaminant models, but the supporting theory is continuously evolving and more experimental validation exercises are being carried out.

How is it solved today, and by whom? The measurement science to simulate whole-building particle transport in buildings, based on a comprehensive treatment of the relevant transport phenomenon, does not currently exist. Particle transport modeling is currently handled by implementing a subset of transport phenomena in detailed computational fluid dynamics (CFD) models or with less detailed models that do not fully consider all the relevant particle transport processes. Neither of these approaches has been fully incorporated into whole building models. Current building models do consider bulk removal mechanisms such as filtration, outdoor-to-indoor penetration, and deposition, but only as first-order effects. Important research is being conducted at a variety of institutions into other critical mass transport mechanisms including Penn State, Syracuse, LBNL and EPA, but these results need to be evaluated technically before they are implemented in indoor contaminant models.

Why NIST? BFRL has conducted numerous experimental and modeling studies of indoor particulate transport that have contributed to the relevant measurement science. In addition, BFRL has developed one of the most widely used predictive tools to analyze multizone building airflow and contaminant transport in the fields of CBR analysis, smoke management system design, ventilation-related energy analysis and indoor air quality. These tools are being advanced to meet the evolving technological needs of those members of the building industry that continue to rely on these critical solution-enabling tools. This project fits under the *Measurement Science for Net Zero Energy, High-Performance Buildings* strategic priority for its indoor environmental health aspects and aligns well with the energy performance aspect of the *Net Zero Energy* and the *Life Cycle Performance*. The CBR and fire-related capabilities of this project also relate to the *Disaster Resilient Structures* and *Innovative Fire Protection* priorities.

Approach:

What is the new technical idea? The main technical idea is to enhance NIST's multizone modeling tools to incorporate more complete particle transport using the latest available research in the field[2]. For example, one of the most immediate modeling needs currently being studied is particle resuspension mechanisms associated with occupant activity. In addition, a means to define particle distributions within the model and account for changes in these distributions is also needed, as opposed to current approaches that consider each particle size in isolation. These distributions are affected by various phenomena including agglomeration of particles to form

larger particles as well as opposite effects, such as evaporation of liquid aerosol droplets. Particle filtration is another area where the multizone model needs to be improved through the implementation of more detailed filter models that account for changes in efficiency and fan performance as a result of filter loading, bypass, breakthrough and environmental effects such as relative humidity. In addition to these enhancements to existing multizone modeling capabilities, this project will also consider micro-scale issues by developing particle transport enhancements to computational fluid dynamic (CFD) models. This work is particularly important given the recent implementation of a combined multizone/CFD capability that is required for the analysis of many critical problems, particularly in the CBR arena.

Why can we succeed now? Advancements have been made in the understanding of particle transport, however these models have not been implemented within the simulation tools that are generally available to practitioners. There is a strong demand for these detailed models based on efforts with DHS, EPA and NIOSH to develop validated biosampling plans for finding building contaminant sites and clearing buildings after decontamination efforts. BFRL has strong building simulation capabilities to meet these needs as well as access to world-class resources on particle transport within other BFRL divisions as well as CSTL.

What is the research plan? The initial phase of this project will consist of a review of particle transport theory in the areas of resuspension, size and mass distributions, agglomeration, evaporation, diffusion, deposition, filtration and penetration. This review will identify those transport phenomena that are deemed most relevant to characterizing transport and exposure in the indoor built environment and most mature for incorporation into building modeling tools. Along with the theoretical review, a review of existing experimental results will be performed to identify areas where model validation data are available and key model input parameters have been characterized. This review will also identify areas where more experimental work is needed in the future. As a result of this review effort, those transport phenomena that have been sufficiently well-characterized will be incorporated into NIST's combined multizone/CFD building airflow and contaminant modeling tool.

It is anticipated that implementation of various aspects of particle behavior into CONTAM will vary in levels of complexity and effort. Some existing models of particle resuspension could be readily implemented to fulfill the more immediate needs of CBR modelers[5], and therefore will be carried out in FY2009 in the multizone portion of ContamX, i.e., the simulation engine of CONTAM. Once the basic method is established within ContamX, the user interface will be modified to enable the general use of the resuspension capabilities including interaction with occupant transport features of CONTAM. Also, in FY2009, particle transport modeling will be implemented in the CFD portion of the combined multizone/CFD version of ContamX. This capability will include non-reactive particles that are influenced by inertia, hydrodynamic drag

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[5] Hu, B., et al., *Modeling Particle Dispersion under Human Activity Disturbance in a Multizone Indoor Environment.* ASCE Journal of Architectural Engineering, **13**, 4, (2007).

and gravitational settling forces. To the extent possible, consideration will be given to implementing duct deposition and aerosol droplet modeling with evaporation.

BRFL will be focused on extending the capabilities of the phenomenon implemented and verifying/validating the models implemented. Validation and verification will include cross-model comparison with other modeling tools and experimental data sets including particle transport data obtained in the NIST Manufactured IAQ Test House and the IAQ Test Chamber in Building 226. Attention will be given to the usability of the new capabilities by the design and analysis community including consideration of leveraging other BFRL-developed software such as SmokeView to visualize results obtained with CONTAM.

Recent Results:

Outcome: CONTAM enhancements have enabled integrated into the High Fidelity Pentagon Model for the Pentagon Force Protection Agency, including the support of very large building models, reductions in airflow calculation time, and real-time data transfer during simulations.

Output: Dols, W.S., Persily, A.K. A Software Tool for Analyzing Building Airflow And Airborne CBR Agent Concentrations. Invited presentation at 2008 International Joint Topical Meeting: Emergency Management & Robotics for Hazardous Environments

Output: Wallace, L. Fang, W., Howard-Reed, C. 2008. Ultrafine particles from 2 nm to 64 nm generated by a gas stove and electric toaster oven: Size-resolved coagulation and emission rates. 11th International Conference on Indoor Air Quality and Climate.

Standards and Codes: This project is expected to contribute to the development of biosampling standards being developed by AOAC (Association of Analytical Communities) International and ASTM.