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# Computer modeling of multiscale fluid flow and heat and mass transfer in engineered spaces

Qingyan (Yan) Chen[a,*], Zhiqiang (John) Zhai[b], Liangzhu (Leon) Wang[a]

[a]*School of Mechanical Engineering, Purdue University, 585 Purdue Mall, West Lafayette, Indiana 47907-2088, USA*

[b]*Department of Civil, Environmental, and Architectural Engineering, University of Colorado at Boulder, UCB 428, ECOT 441, Boulder, CO 80309-0428, USA*

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**Abstract**

Design and analysis of fluid flow and heat and mass transfer in engineered spaces require information of spatial scales ranging from $10^{-7}$ m to $10^{3}$ m and time scales from $10^{-1}$ s to $10^{8}$ s. The studies of such a multiscale problem often use multiple computer models, while each of computer models is applied to a small range of spatial and time scales. Accurate solution normally requires exchanging information between a macroscopic model and a microscopic model that can be done by coupling the two models. With the approach, it is possible to obtain an informative solution with the current computer memory and speed.

This paper used a few examples of fluid flow and heat and mass transfer in engineered spaces to conclude that a coupled macroscopic and microscopic model is likely to have a solution and the solution is unique. A stable solution for the coupled model can be obtained if some criteria are met. The information transfer between the macroscopic and microscopic models is mostly two ways. A one-way assumption can be accepted when the impact from small scale on large scale is not very significant.


*Keywords:* Multiscales; Computer modeling; Macroscopic; Microscopic

## 1. Introduction

“Engineered spaces” are any enclosed environments that are created to provide appropriate conditions and functionality for human and animal habitation. The conditions include thermal comfort, air quality, visual comfort, and acoustic comfort, etc. Examples of engineered spaces are commercial, institutional, and residential buildings; healthcare facilities; sport facilities; manufacturing plants; animal facilities; transportation vehicles (planes, trains, ships, and automobiles); and enclosed spaces for extreme environments (submarines and extraterrestrial vehicles). Although these enclosed spaces differ profoundly in terms of their shapes, functions, and surrounding environments, they are naturally or artificially maintained with appropriate conditions for habitation. The conditions in engineered spaces are always related to the surrounding environments, such as atmospheric environment, ocean, and universal space. The creation and maintenance of appropriate conditions in engineered spaces share many of the same technologies. For example, a computational fluid dynamics (CFD) program can be used to study airflow in different engineered spaces for study and design of air temperature, relative humidity, air velocity, and air quality. However, the spatial scales vary from $10^{-7}$ m to $10^{3}$ m and time scales from $10^{-1}$ s to $10^{8}$ s.

If an office building is used as an example, the study of air quality would require understanding movement of particulate matters from 0.1 μm ($10^{-7}$ m) to 100 μm ($10^{-4}$ m). The study of thermal comfort needs to know airflow and heat transfer in wall boundary layer from 1 mm ($10^{-3}$ m) to 10 cm ($10^{-2}$ m) thick and a spatial resolution from 10 cm ($10^{-2}$ m) in a room and to 100 m ($10^{2}$ m) for a whole building. Since outdoor environment can have a significant influence on the interior environment of the building, the inclusion of building proximity of several street blocks into the study will bring the scale to a kilometer ($10^{3}$ m). By looking at the time scales, the study of thermal comfort would need turbulence intensity of airflow that is as small as a few Hz ($10^{-1}$ s). The cycle of human

* Corresponding author. Tel.: +1 765 496 7562; fax: +1 765 496 7534.
*E-mail address:* yanchen@purdue.edu (Q. Chen).

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breathing is in a scale of a second or two ($10^0$ s). The time constant from airflow in the office can be in the order of $10^1$ s from a fan to $10^3$ s without mechanical ventilation. Depending on the thermal mass in the building, the time constant for heat transfer through building structure is around $10^3$–$10^4$ s. Thermal comfort study will need to understand the impact of outdoor climate that has a time scale of a day ($10^5$ s) to a year ($10^8$ s).

For such a complicated multiscale problem, solving all the information needed for all the scales with a detailed microscopic model may not be efficient (E and Engquist, 2003). For example, CFD simulation of microscopic behavior, such as particle dispersion in a room, is too inefficient to be used in full detail for an entire building. On the other hand, we may be only interested in the macroscopic behavior of the engineered space, such as air quality between two zones in the building. Although the microscopic behavior and macroscopic behavior are linked, CFD is invalid in some parts of the computational domain (such as airflow through cracks between the two zones). Even if CFD can be used, it would require a computer with a huge memory and several months of computing time if CFD simulation is applied to the full spectrum of the spatial and time scales. Basic strategy is to use the detailed microscopic model as a supplement to provide the necessary information for extracting the macroscale behavior of the engineered space through a different model. If this is done properly, the combined macro–micro modeling technique will be much more efficient than solving entire system with the detailed microscopic model (E and Engquist, 2003). This approach has become an essential part of computational science and engineering.

Thus, a multiscale problem in engineered spaces needs multiple computer models. Each of computer models is applied to a small range of spatial and time scales. With the approach, it is possible to obtain information needed with the current computer memory and speed. The information for the whole spectrum of the spatial and time scales is obtained by transferring critical information between two computer models that links two consecutive scales.

There are a few significant questions on such an approach. For example, do they still have a solution when they are coupled? If a solution exists, is it unique? Will the coupling lead to a stable and converged solution? Will the information transfer between the two computer models one way or two ways? This paper tries to answer these questions through a few examples.

## 2. Basic equations

Before we start to answer the questions, this section gives a brief description of two microscale CFD models and two macroscale models–an energy simulation (ES) model and a multizone airflow network model. All of the models are widely used in practice for analyzing and designing engineered spaces.

### 2.1. Governing equations for CFD

A CFD model solves a set of conservation equations that govern flow and heat and mass transfer in engineered spaces. The model has become an indispensable tool for gathering information to be used for design, control and optimization of engineered spaces. CFD can be divided into Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and the Reynolds Averaged Navier–Stokes equations with turbulence models (RANS modeling). DNS, which simulates all the scales of flow eddies, would require a fast computer that does not currently exist, and would take years of computing time for applications in an engineered space. Only LES and RANS modeling are appropriate with current computer power and memory so that they are used as microscale CFD models in this investigation.

RANS modeling separates all spatial parameters, such as velocity and temperature, into their mean and fluctuating components and the fluctuating components are only predicted with time-averaged root-mean-square (rms) values. Thus, RANS modeling solves only the mean components. For time-averaged and incompressible buoyant flow, the basic RANS equations are the continuity equation:

$$\frac{\partial(\rho U_i)}{\partial x_i} = 0 \tag{1}$$

and the momentum equations:

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial(\rho U_j U_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \mu\frac{\partial^2 U_i}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}(\rho\tau_{ij,t}), \tag{2}$$

where $\tau_{ij,t}$ are the eddy (turbulent) stresses that are modeled through a turbulent viscosity, $\mu_t$:

$$\tau_{ij,t} = \frac{\mu_t}{\rho}\frac{\partial U_i}{\partial x_j}. \tag{3}$$

If heat and mass transfer are involved, RANS equation for energy is

$$\frac{\partial}{\partial t}(\rho T) + \frac{\partial}{\partial x_j}(\rho U_j T) = \left(\frac{\mu}{\sigma_T} + \frac{\mu_t}{\sigma_{T,t}}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial T}{\partial x_j}\right) \tag{4}$$

and for species concentration is

$$\frac{\partial}{\partial t}(\rho C) + \frac{\partial}{\partial x_j}(\rho U_j C) = \left(\frac{\mu}{\sigma_C} + \frac{\mu_t}{\sigma_{C,t}}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial C}{\partial x_j}\right). \tag{5}$$

The turbulent viscosity $\mu_t$ in Eqs. (3)–(5) can be obtained with various turbulence models, such as the standard *k–e* model (Launder and Spalding, 1974).

LES is also based on Navier–Stokes equations. LES assumes that flow motion can be separated by large and small scale eddies through a filter. The large scale eddies are directly solved in LES, while the smaller scales are modeled. Since larger scale eddies carry the majority of the energy, they are more important. The smaller scales have been found to be more universal, and hence are more easily modeled. By filtering, one would obtain the continuity equation for the large-eddy motions as

$$\frac{\partial\rho\overline{u_i}}{\partial x_i} = 0 \tag{6}$$

and the momentum equations as

$$\frac{\partial\rho\overline{u_i}}{\partial t} + \frac{\partial}{\partial x_j}(\rho\overline{u_i}\cdot\overline{u_j}) = -\frac{\partial\overline{p}}{\partial x_i} + \mu\frac{\partial^2\overline{u}_i}{\partial x_i \partial x_j} + \frac{\partial\rho\tau_{ij}}{\partial x_j}. \tag{7}$$