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A procedure for verification, validation, and reporting of indoor environment CFD analyses

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ABSTRACT

Computational fluid dynamics (CFD) has been used to help determine the airflow, heat transfer, and chemical species transport in the analysis of indoor environmental conditions as well as a wide range of other HVAC&R applications. The decision to use CFD must be firmly based on realistic expectations of its performance, cost, and effort required. It is necessary to provide instructive materials on how to verify, validate, and report indoor environmental CFD analyses. This paper recommends verifying and validating a CFD code for indoor environment modeling based on the following aspects: basic flow and heat transfer features, turbulence models, auxiliary heat transfer and flow models, numerical methods, assessing CFD predictions, and drawing conclusions. Although the format for reporting of CFD analysis does not necessarily have to be the same, the paper suggests to include all the aspects used in verification and validation for technical readers. It can be simpler for non-technical readers.

NOMENCLATURE

C_p = constant specific heat of air
g = gravitational acceleration
k = thermal conductivity
k = thermal conductivity
L = characteristic length, such as room height or diffuser height
S_ϕ = source or sink
t = time
U = air velocity

Greek symbols

β = thermal expansion coefficient
Γ_ϕ = exchange coefficient
ΔT = temperature difference in an indoor space
ε = dissipation rate of turbulent energy

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ν =molecular viscosity of the fluid
ρ = air density
ϕ = 1 for mass continuity
$\phi = U_j$ (j = 1, 2, and 3) for three components of momentum (U, V, and W)
ϕ = T for temperature
ϕ = C for species concentrations

INTRODUCTION

Computational fluid dynamics (CFD) has been used to help determine the fluid flow, heat transfer, and chemical species transport in the analysis of indoor environmental conditions as well as a wide range of other HVAC&R applications (Ladeinde and Nearon 1997). It has also been used in optimizing the building environment design, reducing the initial and operating costs of the mechanical systems used in the building, and increasing the productivity of the building occupants. Recent advances in computing power and commercial CFD software available to building mechanical engineers make it possible to start using this tool. However, the decision to use CFD must be firmly based on realistic expectations of its performance, cost, and effort required (Martin 1999). It should also be noted that using CFD does not necessarily ensure accurate results (Baker and Gordon 1997, Chen 1997) and involves engineering judgement (Post 1994), and this leads to the desire for developing instructive materials on how to verify, validate, and report indoor environmental CFD analyses. The verification aspect is needed to make sure that relevant physics of the problem are being properly addressed. The validation aspect is needed to demonstrate that the CFD user can successfully model problems for which either experimental data or reliable semi-empirical correlations are available. The reporting aspect is needed for CFD users to communicate with others on the pertinent details of how the analysis was performed and what the results were.

Other engineering professional organizations, including the American Society of Mechanical Engineers (ASME) and the American Institute of Aeronautics and Astronautics (AIAA), have recognized the need for guidance on performing CFD calculations and have already provided guidance to engineers in their disciplines (Freitas 1993, AIAA 1998). Previously within the ASHRAE area, efforts have been made to set forth guidelines for the use of CFD for modeling atria (Schild et al. 1995, Chow 1999) and for the validation of CFD procedures for room air motion prediction (Baker and Kelso 1990). Additionally, there are regularly forum, seminar, and technical symposia at recent ASHRAE meetings related to advancing the use of CFD.

This paper is intended to help building engineers correctly and effectively perform indoor environmental modeling using CFD by defining the steps necessary to verify, validate, and report CFD analyses in relevant applications.

DEFINITIONS OF CFD, VERIFICATION, VALIDATION, AND REPORTING OF RESULTS

What is CFD? In indoor environment modeling, CFD is quantitatively predicting thermal-fluid physical phenomenon in an indoor space. Very often, the physical phenomena are complicated with simultaneous heat flows (e.g. heat conduction through the building enclosure, heat gains from heated objects indoors, and solar radiation through the building fenestration), phase changes (e.g. condensation and evaporation of water contents), chemical reactions (e.g. combustion in case of a fire), and mechanical movements (e.g. fans and occupant movements).

The airflow, convective heat transfer, and species dispersion in the indoor environment are controlled by the governing equations of mass, momentum, and energy (or Navier-Stokes Equation) that can be expressed in a common form in Equation (1). The variable ϕ represents any of the predicted quantities such as air velocity, temperature, or species concentration at any point in the three-dimensional space. The equation refers to the change in time of a variable at a location is equal to the amount of the variable flux (i.e. momentum, mass, thermal energy).

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x_j}(\rho U_j \phi) = \frac{\partial}{\partial x_j}(\Gamma_\phi \frac{\partial \phi}{\partial x_j}) + S_\phi \qquad (1)$$

Transient + Convection = Diffusion + Source

The governing equations remain the same for all indoor environment applications of airflow and heat transfer, but the boundary conditions will change for each specific problem. For example, the layout of a room may be different, or the speed of the supply air may change, and these changes would be implemented through a different set of boundary conditions. In general, a boundary condition defines the physical problem at specific positions.

Since these partial differential equations are coupled together, they must be solved simultaneously. There are no analytical solutions of them available for indoor environment modeling. Computer based numerical procedures are the only means of generating complete solutions of this set of equations.

An engineer (or CFD user) interprets a specific problem of the indoor environment through mathematical form of the conservation law and the information about the specific problem (boundary conditions). These mathematical equations are a conceptual model. The CFD code (i.e. software) embodies the mathematical equations and directs the computer hardware to perform the calculations. Then the engineer inspects and interprets the computed results for the problem. Figure 1 shows such a process.

It is hoped that the CFD simulations should generate reliable results for the problem. However, there is presently little agreement on procedures for assessing the credibility. The principles for assessing credibility are the verification, validation, and reporting of results. AIAA (1998) defines verification as “The process of determining that a (physical/mathematical) model implementation accurately represents the developer’s conceptual description of the model and the solution on the model” and defines validation as “The process of determining the degree to which a (CFD) model is an accurate representation of the real world from the perspective of the intended uses of the model.”

The verification step is done to ensure that a CFD code can accurately and correctly produce a solution for the mathematical equations used in the conceptual model. The verification does not imply that the computational results of a user’s simulation represent the physical reality. Generally, the verification process is done during the CFD code development. Considering the fact that very few people who do indoor environment analysis develop CFD codes, this manual focuses mostly on CFD code applications, not code development. In addition, there is usually limited time and budget available for indoor environment simulation, which requires that the verification and validation should be realistically achievable. Therefore, this manual was developed using refined definitions of the three steps of verification, validation, and reporting of results and includes the following:

- The *verification* identifies the relevant physical phenomena for the indoor environmental analyses and provides a set of instructions on how to assess whether a particular CFD code has the capability to account for those physical phenomena.

- The *validation* provides a set of instructions on how one can demonstrate the coupled ability of a user and a CFD code to accurately conduct representative indoor environmental simulations with which there are experimental data available.
- The *reporting of results* provides a set of instructions on how to summarize the results from a CFD simulation in such a way that others who see the results can make informed assessments of the value and quality of the CFD work.

Therefore, verification cases should represent physical realities, although the cases can be very simple containing only one or more flow and heat transfer features of the complete system. The validation cases should be close to reality and include the flow and heat transfer characteristics that need to be analyzed, although approximations may be used in the validation.

This paper provides a manual for the verification, validation, and reporting of CFD results, but its intent is not to develop standards. The extent of CFD's capability in modeling has not yet developed to the point where standards can be written (AIAA 1998).

VERIFICATION

CFD code is more than just a numerical procedure of solving the governing equations. One should be aware of the capabilities of CFD in modeling an indoor environment. CFD can be used to solve fluid flow, heat transfer, chemical reactions, and even thermal stresses. Unless otherwise implemented, CFD does not solve acoustics and lighting, which are also important parameters in indoor environment analysis. Different CFD codes have different capabilities. A simple CFD code may solve only laminar flow, while a complicated one can handle a flow far more complex, such as a compressible flow.

The basic physical phenomena of the indoor environment are the airflow, heat transfer (conduction, convection, and radiation), mass transfer (species concentrations and solid and liquid particulates), and chemical reactions (combustion). Therefore, the first step of verification is to identify benchmark cases with one or more flow and heat transfer features of those basic phenomena. Most indoor airflows are turbulent, due to the high Rayleigh (Ra) number and sometimes high Reynolds (Re) number. The Ra and Re numbers are defined as

$$\mathrm{Ra} = \beta g \Delta T L^2 / \nu k \qquad (2)$$

$$\mathrm{Re} = UL / \nu \qquad (3)$$

In some regions of an indoor space, the airflow can be laminar or weakly turbulent. The overall flow features are often considered as turbulent. Turbulence modeling approximations have to be made for CFD to solve the flow fields. These approximations will in turn require more complex numerical schemes so that a converged solution can be achieved. There are questions regarding the ability of a CFD code to simulate airflow in an indoor environment and the fidelity of the computer model to the physical realities. The prediction of physical phenomena in an indoor environment may require auxiliary flow and heat transfer models. It is necessary to assess whether a CFD code can be used to simulate these physical phenomena in an indoor environment. Special attention needs to be paid to the following aspects:

- Basic flow and heat transfer (convection, diffusion, conduction, and/or radiation)
- Turbulence models
- Auxiliary heat transfer and flow models
- Numerical methods
- Assessing CFD predictions

Basic flow and heat transfer

Indoor environment analyses should first study the flow and heat transfer features, which include convection, diffusion, conduction, and/or radiation. Convection involves mass and energy exchange due to flow and temperature gradient. The cold or warm airflow from a diffuser is a typical example of convection. Diffusion can take place together with convection, due to turbulent motion and molecular movement. For example, environmental tobacco smoke may diffuse from one location to another. Conduction happens in solid materials. Heat loss from room air through walls in a cold winter day is an example of conduction. Radiation occurs between two objects with different temperatures that are separated by a transparent medium, such as air. The heat exchange between a radiator and the surrounding walls is mainly by radiation. Whether a CFD code can be used to simulate an indoor environment depends on the flow and heat transfer features. For an indoor space with a baseboard heater, a CFD code capable to solve natural convection flow may be sufficient. If a radiator replaces the baseboard heater, a radiation model is needed in the CFD code. When the heat transfer through the walls needs to be considered, the CFD code should have a conjugate heat transfer feature. When the room uses a duct to supply fresh air, the room airflow turns to mixed convection, which requires the capability of mixed convection simulation. For indoor air quality studies, the CFD code should be able to solve species concentrations. The more real the space is, the more complex the flow and the heat transfer are. The CFD user must first verify whether the CFD code is capable of characterizing the physics of the indoor environment to be analyzed.

For a user to verify the capability of a CFD code in simulating the indoor environment of interest, the user should first review the code manual and fundamentals. Many CFD codes also provide libraries and examples to which the code has been successfully applied. The user may also discuss the indoor environment application with the code developer to make sure that the physical models required for the application are all available.

However, even if a CFD code has been proven to be capable of simulating the physical phenomena in the indoor environment by other users, repeating the verification will be helpful. This is because a successful simulation of indoor environment relies on the joint function of the user and the CFD code.

The hands-on verification usually starts with the simplest cases. These cases contain only one or two flow features and are well tested by other people. The uncertainties and errors in these cases are thus minimal. After a successful verification, simulations can be further carried on for cases closer to reality. These cases may contain many key features of physical phenomena in an indoor space. The Reynolds numbers or Rayleigh numbers can then be similar to those in reality.

Often, the data available for verification are from high precision experimental measurements. The quantity and quality of the experimental data are usually accompanied by quantified errors. They are generally accurate, and have few human errors. These cases cover a large area of interest within the CFD community, and are widely cited and used for testing CFD simulations. In addition, these experimental data contain detailed information, such as boundary conditions and initial conditions. These cases are usually two-dimensional.

Note that the verification should be done for one or more cases. Different cases represent different flow characteristics. Ideally, the verification should be done for all the flow features. In practice, however, two to three important cases may be sufficient for most indoor environmental analyses.

Turbulence models

With a verification case in mind, the next step is to identify a suitable turbulence model. If the Navier-Stokes equations are solved without using any approximations in turbulence simulation, the approach is called direct-numerical simulation. Successful prediction of a turbulent flow with the direct-numerical simulation method requires a very fine numerical resolution to capture all the details of the turbulent flow. The smallest eddy size in the turbulent flow is of the order of the Kolmogorov length scale, l

$$l = \nu^3/\varepsilon \tag{4}$$

For most indoor airflow, the Kolmogorov length scale is around 0.01 to 0.001 m. The corresponding grid number, N_{DNS}, needed in a direct-numerical simulation is

$$N_{DNS}^3 = \left(\frac{L}{l}\right)^3 \mathrm{Re}_l^{9/4} \tag{5}$$

which, for a small office, is in a range of 10^{15} to 10^{18}, where L = 3 m and Re = 5,000. A high-end desktop computer, at present, may handle a grid number of 10^8. In addition, it will take years of computing time in order to reach a solution. It is clear that applying direct-numerical simulation to indoor airflow is not realistic at present for designers. Therefore, a successful simulation of turbulent flow in an indoor space must use approximations, namely, turbulence models.

By using turbulence models, it is feasible to compute the airflow in the indoor environment with the capacity and speed of present computers. The turbulence models can be divided into two groups: large-eddy simulations (LES), and turbulent transport models (or Reynolds averaged Navier-Stokes equation modeling, RANS).

LES divides the turbulent flow into two parts: large-scale motion and small-scale motion. Large-scale motion is calculated in LES, while the small-scale motion needs to be modeled because of its effect on the large-scale motion. The most important aspect in application of LES is to use a suitable subgrid scale model for the simulation. The accuracy and efficiency of the subgrid scale model will determine the correctness and usefulness of the LES that is performed.

As LES models have only one or no empirical coefficient, few modeling assumptions are involved. However, LES always solves three-dimensional, time-dependent flow, although the flow can be steady. It calculates a mean of the time-dependent flow fields to obtain the steady-state solution. Therefore, it requires a great deal of computing time. To date, only a few LES applications have been performed for indoor environment modeling due to the high computing costs (Davidson and Nielsen 1996, Emmerich and McGratten 1998, Zhang and Chen 2000). The LES could be a powerful modeling tool in the near future.

RANS modeling solves the mean flow variables by using turbulence transport models. Depending on how the Reynolds stresses are modeled, turbulent transport models are further classified as eddy-viscosity models and Reynolds-stress models. An early and popular eddy-viscosity model is the k-ε model from Launder and Spalding (1974). Low-Reynolds-number models and other variations of k-ε model all fall in this class. A basic Reynolds-stress model is the one summarized by Launder (1989). The Reynolds-stress models are superior to the eddy-viscosity models, because the Reynolds-stress models do not use the Bousinessq approximation. However, there is a penalty in terms of model complexity, computing requirements, and numeric algorithm stability with the Reynolds-stress models.

This manual does not intend to help a user in choosing an appropriate turbulence model. Nielsen (1998) showed how to select a suitable turbulence model. He concluded that a simple zero-equation model can be useful for provisional studies, a k-ε model can be used for stratified flows, a low Reynolds number k-ε model is need for transport processes close to surfaces, and an LES can provide the highest level of flow information. Others have also compared different turbulence models (Murakami et al. 1996, Chen 1995 and 1996, Murakami 1998). In general, complex turbulence models, such as Reynolds stress models, produce better accuracy. However, there are penalties in terms of numerical stability and computing time. In most cases, simple models, such as the standard k-ε model (Launder and Spalding 1974) and re-normalization group k- ε model can provide satisfactory results for most indoor air simulations.

Theoretically, LES, Reynolds stress models, and eddy viscosity models can all be used to simulate turbulent flow and heat transfer in an indoor space. However, understanding the differences between these models is the key to identifying a suitable one for an indoor environment analysis.

LES is suitable for transient simulation because it always calculates the flow in a transient form. LES uses a finer grid distribution than is typically used with the RANS equations, which will dramatically increase the computing time. Unlike the RANS equations, the accuracy of LES results depends on the grid resolution. The finer the grid, the more accurate the results. Therefore, for steady airflow simulations, RANS equations with turbulent transport models are recommended. However, the fine grid distribution allows modeling of the flow as an isotropic turbulence within a grid cell. Since complete statistical theory of isotropic turbulence is available, the approximations used in subgrid-scale model of LES introduce little errors when the grid resolution is sufficiently fine. As a result, LES results should be better than those obtained from the RANS equations with turbulent transport models. LES also provides more detailed flow information. Please note that most CFD codes available on the market at present are based on RANS equations with turbulent transport models. These codes can also be used for transient flows. When both the LES and turbulent transport models are available in a CFD code, the latter requires much less computing time and, therefore, can be very appealing for indoor environment design. The user has to make a decision based on the problem to be solved.

In general, the eddy viscosity models are accurate for simple airflows and the Reynolds stress models are needed for complex flows. Complex flow exists in a flow domain with complex geometry, such as room and air supply diffuser geometry. As many CFD studies compare different turbulence models, users may look up the literature for reported CFD studies that are close to the case to be studied. It is known that the k-ε model is inaccurate for flows with adverse pressure gradient and that poses a serious limitation to its general utility. In case studies of model comparison for the case are not available, the user should start from simple and popular models, such as the standard k-ε model (Launder and Spalding 1974). If the model does not provide satisfactory results, a more complicated model should be tested. The effort of CFD code vendors has made the selection of different turbulence models as easy as a simple click on the computer screen.

Auxiliary heat transfer and flow models

The indoor environment consists of very complicated physical phenomena. Radiative, conductive, and convective heat transfer occurs simultaneously in almost all types of indoor environment. Sometimes the physical phenomena include also combustion, participating media radiation, and particle transport in multi-phases (air-liquid, air-solid, and air-liquid-solid). It is important to verify whether the above-mentioned physical phenomena can be modeled by a CFD code.

It is suggested that the verification of the auxiliary models should be separated from that of a turbulence model. This would reduce the possibility of an error. According to AIAA (1998), an error is “a recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge." A complex problem may be verified by separating it into several components for which analytical solutions may be available. For example, a combined conductive, convective, and radiative heat transfer process can be verified by separating it into a conductive and radiative problem, and a convective problem. The two problems can then be verified by the relevant analytical solutions. Another example is liquid particle trajectory in indoor air quality simulations in which condensation, evaporation, and collision are all involved in addition to the strong interaction with the airflow turbulence. The physical phenomena should be verified separately.

The recommended verification does not ensure the correctness of the combined process. Therefore, uncertainty exists in the combined process. The uncertainty is a potential deficiency in any phase or activity of the modeling process due to lack of knowledge and there are no highly accurate solutions available. This may be remedied in the validation process.

Numerical methods

A CFD code solves the turbulence flow and auxiliary heat transfer models by the discretization of the continuous space and time (if transient) into finite intervals. The variables are computed at only a finite number of locations, the so-called grid points. This means that the continuous information contained in the solution of the differential equations is replaced with discrete values. The common discretization methods used in CFD technique are the finite-difference, finite-volume, and finite-element methods. The space can be discretized in orthogonal or non-orthogonal coordinate systems. The numerical grid can be structured or unstructured to meet the requirements of different applications. Unstructured meshes are usually body-fitted and structured meshes can be either body-fitted or Cartesian. For example, Cartesian coordinates are perfect for an empty rectangular room, while to accurately simulate heat transfer between a human body and the surrounding air, one may need a body-fitted mesh system. When a Cartesian mesh system is used for sloped or curved surfaces, the true geometry is not represented in the calculation. This would introduce an error. Thus, if the user intends to use CFD for sloped or curved surfaces, he/she would perform verification on similar geometries rather restricting himself/herself to empty rectangular rooms.

A user can verify different discretization schemes by comparing the results obtained from two different schemes. For example, if one would like to verify an unstructured grid system, Cartesian coordinates can be used as a reference. The geometry of the case should be simple, such as a rectangular room. Then, the two schemes should generate the same results. If the CFD code has only one grid system, the discretization scheme verification can be combined with the CFD model verification.

Another important action in verification testing is systematically refining the grid size and time step. Since CFD discretizes partial differential equations into discretized equations, this introduces an error. The verification on grid size and time step is to reduce the error to a level acceptable for the particular application. The time step applies only to transient flow simulation. Therefore, it is not sufficient to perform CFD computations on a single fixed grid. The difference in grid size and time step between two cases should be sufficiently large in order to identify the differences in CFD results. The common way is to repeat the computation by doubling the grid number and compare the two solutions (Wilcox 1993). The study is very important to separate numerical error from turbulence-model error, since no objective evaluation of the merits of different turbulence models can be made unless the discretization error of the numerical algorithm is known (Wilcox 1993). The geometry of an indoor space can be very complicated.

The computer speed and capacity available for engineers are still not sufficient for simulating an indoor environment with very fine grid sizes (over a few million grids) and time steps (tens thousands). Verification involves estimating the discretization error of the numerical solution. Theoretically, when the grid size and time step approach zero, the discretization error of the numerical solution becomes negligible. For LES, when the grid size and the time step become small, the flow in the subgrid scale is isotropic, and the LES results become more accurate. When the grid size is much smaller than the Kolmogorov length scale, the LES turns into a direct-numerical simulation.

The last step of the verification process is related to numerical schemes, iteration, and convergence. A numerical scheme plays an important role in a CFD code in order to obtain a fast, accurate, and stable solution. A higher-order differencing scheme is expected to be more accurate results than a lower-order scheme for simple cases, such as those suggested for turbulence model verification. However, one should be aware of the limitations of various differencing schemes. For example, the central differencing scheme, which is accurate to the second order, is employed for small Peclet numbers ($Pe < 2$), and the upwind scheme, which is accurate to the first order (but accounts for transportiveness), is employed for a high Peclet number. The Peclet number, the ratio of convection over conduction, is defined as

$$Pe = L\ U\ \rho\ C_p / k \qquad (6)$$

The solution algorithms used in the CFD codes can be quite different. They range from the SIMPLE in conventional program with iteration to the Fast Fourier Transformation used for solving the Poisson pressure equation in LES without iteration. The iteration is normally needed in two situations: (1) globally for boundary value problems, i.e., over the entire domain; and (2) within each time step for transient physical phenomena. Criterion can be set to determine if a converged solution is reached, such as a specified absolute and relative residual tolerance. The residual is the unbalance of those variables solved, such as velocities, mass flow, energy, turbulence quantities, and species concentrations. For indoor environment modeling, a CFD solution has converged if:

Residual for mass = The sum of the absolute residuals in each cell / the total mass inflow < 0.1%
Residual for energy = The sum of the absolute residuals in each cell / the total heat gains < 1%

Similar convergence criterion can be defined for other solved variables, such as species concentration and turbulence parameters. Note that for natural convection in a room, the net mass flow is zero. Therefore, one can conclude that a convergence has been reached if there is little change (no change in the 4th digit) on the major dependent variables (temperature, velocities, and concentrations) within the last 100 iterations. However, a small relaxation factor can always give a false indication of convergence (Anderson et al. 1984).

In order to obtain stable and converged results, the iteration procedure often uses relaxation factors for different variable solved, such as under-relaxation factors and false-time-steps. The under-relaxation factors differ a little bit from the false-time-steps, but there is no substantial differences.

Assessing CFD predictions

This section should provide in detail both qualitative and quantitative comparison of CFD results with data from experiment, analytical solutions, and direct numerical simulations. All the error analyses should be detailed in this section as well. The results present in this section should serve as a basis to judge whether the CFD code can be used for indoor environment modeling.

Although this manual divides the verification into several parts, they are integrated in many cases. The turbulence model and numerical technique must work together in order to obtain a correct CFD prediction for the flow features being selected. However, it is necessary to break them down into individual items in some types of verifications, such as in the CFD code developments. Indoor environment designers often use commercial software. It is logical to assume that the codes have been verified during the code development. However, the verifications, if they are performed at all, may have used different flows that are irrelevant to indoor airflow. In addition, a user may not fully understand the functions of the CFD code. It is imperative for the user to "re-verify" the capabilities of a CFD code for indoor environment simulations. This will help the user become more familiar with the CFD code and eliminate human errors in using the code.

In general, the cases used for verification are not company-proprietary or restricted for security reasons. These data are usually available from the literature. It is strongly recommended to report the verification. This is especially helpful in eliminating errors caused by the users, since most CFD codes may have been validated by those cases. There are many examples of failed CFD simulations due to the user's mistakes.

The verification should be done for the following parameters:

- All the variables solved by the governing equations, such as velocity, temperature, species concentrations
- Boundary conditions such as heat flux and mass inflow and outflow rates

With the verification described above, a CFD code should be able to correctly compute the airflow and heat transfer encountered in an indoor environment. The level of the accuracy depends on the criteria used in the verification. If the CFD code failed to compute correctly the flow, the problem may be: (1) the CFD code is not capable to solve the indoor airflows, (2) the CFD code has bugs, or (3) there are errors in the user input data that defines the problem to be solved.

VALIDATION

Validation is the demonstration of the coupled ability of the user and the CFD code to accurately predict representative indoor environmental applications for which some sort of reliable data is available. The validation estimates how accurately the user can apply the CFD code in simulating a full indoor environment problem in the real world. It gives the user the confidence to use the CFD code for further applications, such as a design tool. A CFD code may have solved the physical models that the user selects to describe the real world, however, the results may not be accurate because the selected models do not represent the physical reality. For example, an indoor environment may involve simultaneously conduction, convection, and radiation. A CFD user may misinterpret the problem as purely convection. The CFD prediction may be correct for the convection part, but fails in describing the complete physics involved in the case. It is obviously a problem on the user's side, which the validation process is also trying to eliminate.

The fundamental strategy of validation is to identify suitable experimental data, to make sure that all the important physical phenomena in the problem of interest are correctly modeled, and to quantify the error and uncertainty in the CFD simulation. Since the primary role of CFD in indoor environment modeling is to serve as a high-fidelity tool for design and analysis, it is essential to have a systematic, rational, and affordable code validation process.

Validation is focused on the

- Confirmation of the capabilities of the turbulence model and other auxiliary models in predicting all the important physical phenomena associated with an indoor environment, before applying the CFD model for design and evaluation of a similar indoor environment category
- Confirmation of correctness of the discretization method, grid resolution, and numerical algorithm for the flow simulation
- Confirmation of the user’s knowledge on the CFD code and his/her understanding to the basic physics involved in the indoor environment analysis

Validation procedure

Ideally, validation should be performed for a complete indoor environment system that includes all the important airflow and heat transfer physics and a full geometric configuration. Experimental data for a complete system can be obtained from on-site measurements and the experiments in an environmental chamber. The data usually have a fairly high degree of uncertainty and large errors. The data may contain little information about the initial and boundary conditions. Reasonable assumptions are needed to make a CFD simulation feasible.

The definition of validation used in this manual sounds very similar to that of verification. There are substantial differences. The validation is for a complete flow and heat transfer system or several subsystems that can altogether represent a complete system. However, verification is only for one of the flow aspects found in an indoor environment. The validation procedure is almost same between the verification and validation. The validation procedure involves:

- The complete indoor environment system design for validation
- Turbulence models
- Auxiliary heat transfer and flow models
- Numerical methods
- Assessing CFD predictions
- Drawing conclusions

The procedure will be the same as for verification, and, therefore, will not be repeated here. However, the validation requires analyzing the CFD results and experimental data in order to draw some conclusions for indoor environment analyses.

Very often, experimental data may not be available for a complete indoor environment system. It is acceptable to utilize validations for several subsystems or a less-than-complete system. A subsystem of indoor environment represents some of the flow features in an indoor environment to be analyzed. The overall effect of several subsystems is equivalent to a complete system. For example, a complete indoor environment system consists of airflow and heat transfer in a room with occupants, furniture, and a forced air unit. If a user can correctly simulate several subsystems such as (1) airflow and heat transfer around a person, (2) airflow and heat transfer in a room with obstacles, and (3) airflow and heat transfer in a room with a forced air unit, the validation is acceptable. In the same example, a less-than-complete system for this environment can consist of airflow and heat transfer in a room with an occupant and a forced air unit. The furniture, although it affects the indoor environment, is not as important as the other components. Therefore, the validation with a less-than-complete system is acceptable. In either case, the key is that the validation should lead to a solid confirmation of the combined capabilities of the CFD user and code.

Although the validation is for a complete indoor environment system, it is not necessary to start with a very complicated case if the user has a number of alternatives. Reliability is better:

- For a simple geometry, rather than a complicated one
- For convection, rather than combined convection, conduction, and radiation
- For single-phase flows, rather than multi-phase flows
- For chemically-inert materials, rather than chemically-reactive materials

This is because, for complex physical phenomena in an indoor space, the input data for CFD analysis may involve too much guesswork or imprecision. The available computer power may not be sufficient for high numerical accuracy, and the scientific knowledge base may be inadequate.

The validation of a complete system should be broken down into several steps. The first step will be the setup of the building geometry, followed by placement of the inlets and outlets. The isothermal flow will give an indication of the airflow pattern. The second step will be adding heat transfer. Species concentration, particle trajectory, and others should be considered later. This progressive simulation procedure will not only build confidence in the user at performing the simulation, but will also discover some potential errors in the simulation.

On the other hand, simple and popular models in a CFD code should be considered as the starting point for validation if a CFD code has multiple choices. The starting point can be as basic as:

- Standard k-ε model
- No auxiliary flow and heat transfer models
- Structured mesh system
- Upwind scheme
- SIMPLE algorithm

The way of measuring the accuracy of the representation of the real world is to systematically compare CFD simulations to the experimental data. The indoor environment systems used in validation are usually complicated, and the corresponding experimental data may contain biased errors and random errors. These errors should be reported as part of the validation. In case the errors are unknown, a report on the equipment used in the measurements will be helpful in assessing the quality of the data. Although desirable, it is expensive and time-consuming to obtain good quality data for a complete system. Therefore, reporting the CFD validation of the complete system cannot be overemphasized.

Validation criteria

The criteria for accuracy when conducting a validation depend on the application. Very high accuracy, while desirable, is not essential since most design changes are incremental variations from a baseline. As long as the trends that are predicted are consistent, then less-than-perfect accuracy should be acceptable. The validation process should be flexible, allowing a varying level of accuracy, and be tolerant of incremental improvements as time and funding permit. The level of agreement achieved with the test data, taking into the account measurement uncertainties, should be reviewed in light of the CFD application requirements. For example, validation for modeling air temperature in a fire simulation requires a much lower accuracy than that for thermal comfort study for an indoor environment.

If the validation cases are simple and represent a subsystem of a complex indoor airflow, the validation criteria should be more restrictive than those for the complete system. The criteria can also be selective. For example, if correct prediction of air velocity is more important, the criteria for heat transfer may be relaxed. Although the air velocity and temperature are inter-related, the impact of one parameter over the other may be of second order. This would allow the CFD user to use a fast and less detailed model, such as standard k-ε model, rather than a detailed but slower model, such as low Reynolds number model for heat transfer calculation in boundary layers.

REPORTING OF CFD RESULTS

The reporting of the CFD results involves informatively summarizing the CFD simulation results for an indoor environment, while providing sufficient information on the value and quality of the CFD work. This is an important quality assurance strategy for the CFD analysis of the indoor environment.

When reporting the results, it is better to start with verification and then proceed to validation. In principle, the reporting should include the information discussed in the verification and validation sections, such as

- Experimental design
- CFD models and auxiliary heat transfer and flow models
- Boundary conditions
- Numerical methods
- Comparison of the CFD results with the data
- Drawing conclusions

The reporting format, however, can be flexible. The above recommendation is for preparing report for technical readers. If a report were intended for non-technical readers, only the last two items would be sufficient. The following provides a guide for reporting to technical readers.

Experimental design

The first step in the reporting of CFD results is giving a detailed description of the experimental design including the thermal and flow conditions of the test environment. The information provided should also be sufficiently detailed so that other people could repeat the simulation. It can be as simple as a reference to the literature or a description of the cases in the report. An analysis on uncertainties and errors in the experimental data or a short description of the experimental procedure and equipment should also be included in the report.

Turbulence models and auxiliary heat transfer and flow models

Many popular turbulence models have been widely used and reported in indoor environment applications. It is therefore not necessary to provide detailed formulation about those popular models. CFD contains hundreds of different models of LES and RANS. When reporting CFD results, it is important to specify which turbulence model is used. If the model is not a popular one, detailed information concerning the turbulence model should be presented. It is desirable to provide a brief description why such a model is selected.

Indoor environment analysis may require auxiliary heat transfer and flow models. For example, a building may use porous material as insulation. The heat transfer through the insulation material involves conduction, convection, and radiation. Limited computer resources would not allow detailed simulation of the heat transfer process. A lumped-parameter model may be used to combine the heat transfer processes. This model is important for obtaining accurate

CFD results for the indoor environment. Therefore, it should be described in the CFD analysis report.

Boundary conditions

Accurate specifications of boundary conditions are crucial in CFD modeling of indoor environments. The boundary conditions indicate how the CFD code user interprets the specific physical phenomena into a computer model or mathematical equations, so that a CFD code can be used to solve the phenomena. This interpretation is the part that requires the most skill in CFD modeling. Therefore, a detailed description of the boundary conditions can help others make informed assessments of the quality of the CFD simulation. The boundary conditions should include the following information:

- *Geometry settings*: The geometry setting of a CFD model refers to the size of the computational domain along with sizes and locations of all the solid objects represented in the model. If there is an external wall involved that cannot be considered as adiabatic, the external ambient conditions such as ambient temperature, external radiation temperature and convective heat transfer coefficient need to be reported as well.
- *Inlet*: The airflow from a diffuser greatly affects the airflow pattern in a room. The geometry of a diffuser is very complicated. Approximations are often used in a complete system in order to make the indoor airflow solvable. Therefore, the CFD report should give detailed information on the approximations used in addition to what has been set as the boundary conditions for the inlet. In some situations, the exact location of an inlet may be difficult to identify. For example, air infiltration from the outdoors to an indoor space could be through the cracks of windows and doors. The conditions may be different from one window to another. In addition, the infiltration flow rate can be difficult to estimate because the wind outdoors changes its magnitude and direction over time. Furthermore, the turbulence parameters for the inlet are generally unknown, and should somehow be estimated. Therefore, how these “inlet” conditions are specified should be clearly stated.
- *Outlet*: It is observed that an outlet has little impact on room airflow. However, the conditions set for the outlet can have a significant influence on the numerical stability in many cases. For example, the outlet may become an inlet during the iteration in a calculation. If the outlet temperature is default as 0^{o}C, this could lead to a diverged solution.
- *Walls*: Rigid surfaces in an indoor space, such as walls, ceilings, floors, and the furniture surfaces, are all considered as walls. In the region very close to the wall, the airflow is laminar, and often the convective heat transfer occurs in this region between the flow and the surfaces. Many turbulence models cannot accurately handle laminar sublayer, so ad hoc solutions, such as damping functions, are often employed. The treatment of a CFD code on the wall boundary conditions is of great importance to the accuracy of numerical results. Even if the indoor space is large and the wall impact seems small, it is still important to predict accurately the heat transfer from the walls to room air.
- *Open boundary*: When the area of interest is a part of the indoor space, the computational domain does not have to align with a rigid surface, instead, an “open” boundary can be defined. Depending on the inside and outside pressure difference, air may flow in or out across the open boundary. A CFD report should include such information.

- *Source/sink***:** This is a boundary condition that fixes thermal or dynamic parameters, in a defined region. The thermal and dynamic parameters can be heat flux from a wall to simulate the solar radiation; total heat flow in the occupied zone to simulate the heat dissipation from occupants; momentum source from an operating fan; species generation rate from contaminant sources, etc. The location, size and parameter being specified all need to be described in the report.
- *Coupling between a micro and a macro model*: When an indoor space is large, a CFD analysis may be divided into micro and macro CFD simulations. The micro simulation zooms into a particular area to reveal the details of flow and thermal characteristic in a small scale in comparison with that for the entire indoor space of interest. This allows the use of a finer resolution to examine the details of the flow in that area. The macro simulation is applied to the entire flow system, and may use the results of the micro simulation so that a coarser grid system can be used. Such a coupling is usually a complicated procedure that needs to be detailed in the CFD report.
- *Other approximations*: Approximations are almost always involved when representing the real world in a computer model. For example, when the surface temperature distribution of a heated object is not uniform, the CFD simulation may choose to neglect the temperature variation on the surface. When designing a large stadium, it may not be feasible to simulate each individual spectator. The CFD modeling may combine all the spectators into a human layer. There are numerous examples in indoor environment modeling that need to be approximated in a CFD simulation. All the approximations should be reported.

Numerical methods

It is essential to report the numerical technique used in the CFD analysis of indoor environment. The report can be brief, if the technique is popular and widely available from the literature. The numerical technique includes discretization technique, grid size and quality, time step, numerical schemes, iteration number, and convergence criteria. The report should briefly state why such a numerical technique is used, and how suitable it is to the problem under consideration. It is also important to provide the quality indices of the mesh of a body-fitted coordinate since the mesh quality affects the accuracy of the CFD prediction. Typically, these indices include the normal distances from solid surfaces to the centers of the first adjacent cells, the maximum scale ratios of each two neighboring cells in each coordinate, and the smallest angle of the mesh cells. The first index determines the prediction of boundary layer flows, while the other two indices indicate whether unacceptable numerical errors are introduced into the simulation. The CFD report should also include grid refinement studies. Since the coarse grid introduces more numerical viscosity, grid-refinement study is essentially necessary to achieve a grid-independent solution. Although it may not be realistic to conduct grid refinement for the complete system, such a grid refinement should be conducted for benchmark cases, in order to estimate the errors introduced in the complete system.

If a user has tested the different numerical schemes, the results should be reported. It is always valuable to know the performance of different numerical schemes for indoor environment CFD analysis. Such a report will help to identify whether a numerical scheme or a turbulence model causes a discrepancy between the CFD results and the experimental data.

Iteration number and convergence criteria are interrelated. It is better to use the sum of the absolute residual at each cell for all the variables as convergence criteria. The relaxation method and values should also be reported.

Assessing CFD predictions

Comparing CFD results with experimental data is the most important part of reporting a CFD analysis for an indoor environment. The comparison should be first performed for qualitative values, such as airflow pattern. Then the comparison can be done for the first-order parameters, such as air velocity, temperature, and species concentrations. In general, both CFD results and experimental data have better accuracy for the first-order parameters. The second-order parameters, such as turbulence kinetic energy, Reynolds-stresses, and heat fluxes, are usually associated with greater uncertainties and errors than the first-order parameters in both the CFD results and the experimental data. Therefore, pursuing perfect agreement between the CFD results and the data for the second-order parameters is not necessary.

Very similar to verification, validation should be done for the following parameters:

- All the variables solved by the governing equations, such as velocity, temperature, species concentrations
- Boundary conditions such as heat flux and mass inflow and outflow rates

It is insufficient to describe the comparison between CFD results and experimental data as “excellent”, “good”, “fair”, “poor”, and/or “unacceptable.” For example, a 20% difference can be considered as excellent for a complex flow problem. However, the difference is rather poor if it is for a two-dimensional forced convection in an empty room. Therefore, the comparison should be quantitative. The most useful information obtained from the comparison lies on how to interpret the discrepancies. If there is little discrepancy it is important to know why a turbulence model that uses approximations can predict the physical phenomena so well. The comparison should clearly state the uncertainties and errors of the experimental data, if they are known.

Drawing conclusions

Finally, the report should include the most important findings of the CFD analysis as its conclusions. Those conclusions should have broad applicability to indoor environment simulation. The report may also recommend measures for further improvements in CFD analyses.

CONCLUSIONS

A manual has been developed that describes how to verify, validate, and report indoor environment modeling CFD analyses. Verification involves identifying the relevant physical phenomena for an indoor environmental analysis and assessing whether or not a particular CFD code itself has the capability of accounting for those physical phenomena. Validation involves demonstrating the coupled ability of a user and a CFD code to accurately conduct a simulation of a representative indoor environment. Reporting results involves summarizing the CFD analysis so that others can make informed assessments of the value and quality of the CFD. This manual provides a set of instructions on how best to perform these three steps for a CFD analysis.

The manual recommends verifying a CFD code for the modeling of the physical phenomena in an indoor environment based on the following aspects:

- Basic flow and heat transfer features
- Turbulence models

- Auxiliary heat transfer and flow models
- Numerical methods
- Assessing CFD predictions

Verification is recommended for both developers and users of CFD codes. The developers can use the verification to check the code for bugs, while the users can become familiar with the features and capabilities of the code. Verification should be performed for simple cases with only one or two flow and heat transfer features of the physical phenomena of an indoor environment system.

Validation is applied for:

- Confirming the abilities of the turbulence model and other auxiliary models at predicting all physical phenomena in a particular indoor environment, in order to apply the models for design and evaluation of a similar indoor environment category
- Confirming the discretization method, grid resolution, and numerical algorithm for the flow simulation
- Confirming the user’s ability to use the CFD code to perform an indoor environment analysis

The validation covers the same aspects as those for verification. However, the validation is for a complete indoor environment system or several subsystems that represent the complete flow, heat and mass transfer features in an indoor environment. Although the validation is for a complete indoor environment system or several subsystems, the manual recommends a progressive validation procedure. The CFD model should also be constructed in progressive stages. The sequence should be (1) correctly set up the flow domain and geometry, (2) progressively increase the complexity of the flow and thermal boundary conditions, and (3) than fine tune numerical schemes and convergence criteria.

Although the format for reporting of CFD analysis does not necessarily have to be the same, the report should include all the aspects of verification and validation for technical readers. The report should provide adequate analysis of the results, and clearly state the uncertainties and errors of the experimental data, if they are known. The report should also conclude the most important findings of the CFD analysis. The report may present lessons learned during the CFD analysis, and recommend measures for further improvements. The report for non-technical readers can be much simpler.

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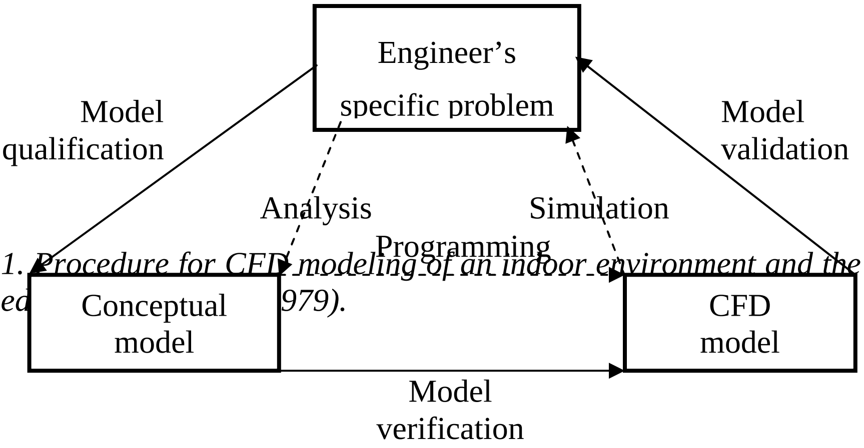

Figure 1. Procedure for CFD modeling of an indoor environment and the corresponding phases (Modified [illegible] 979).