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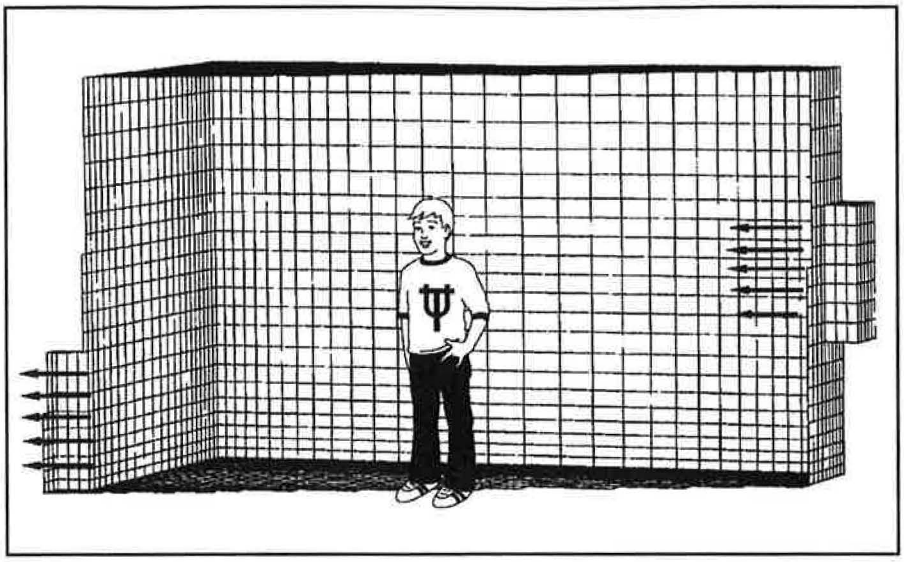

Figure 1a: Scaled "graduate student" provides perspective in this drawing which shows supply and exhaust duct locations for full-scale experiments.

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Computational Fluid Dynamics: A Two-Edged Sword

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Two decades have passed since the first paper [1] was published in the ASHRAE *Transactions* suggesting the use of computational fluid dynamics (CFD) for quantitative prediction of room air motion. CFD is an emerging methodology, with roots in the defense/aerospace industry, wherein a *mathematical model* of fluid flow is converted into a digital computational procedure, yielding numbers that *approximate* the solution of this modeled system, hence the genuine flow state.

Following the lead in Europe and Japan, ASHRAE decided to investigate the use of CFD methodology for predicting air motion. A TRP was let in 1989, leading to organization and completion of ASHRAE Research Project 464 (RP-464) which examined thoroughly the many issues associated with CFD simulation in the indoor room air environment. Results of this research project are published in the ASHRAE *Transactions* [2-5], containing detail on associated mathematical and computer practice issues in technical thoroughness. This Journal article is intended to interpret these and companion results, to help inform the HVAC engineering community on this rapidly advancing technology.

The emergence of Unix workstations, or Pentium PCs, the *windows* environment, and color graphics lends an aura of elegance to the presentation of CFD-produced results. However, beautiful color graphic presentations of velocity vector, temperature and/or contaminant fields can hide distressing factors. (A noted researcher once offered the opinion that CFD stood for "*colorful fluid dynamics*.") Therefore, the engineer in HVAC design must view graphic data presentations with a critical eye, hence insist on assurance of their quality.

Basically, it's a *good* news/*bad* news scenario regarding CFD modeling of room air motion and contaminant transport prediction. CFD methodology has indeed brought bright glimmers of an ability to establish firm *quantitative* data regarding how room air moves. In fact, CFD can predict fluid levels and pressure differences to very low levels, that are essentially impossible to experimentally measure. However, a CFD model constitutes the culmination of a *large number* of *assumptions* and *approximations*, such that the answers produced are essentially *never correct*! Further, it is

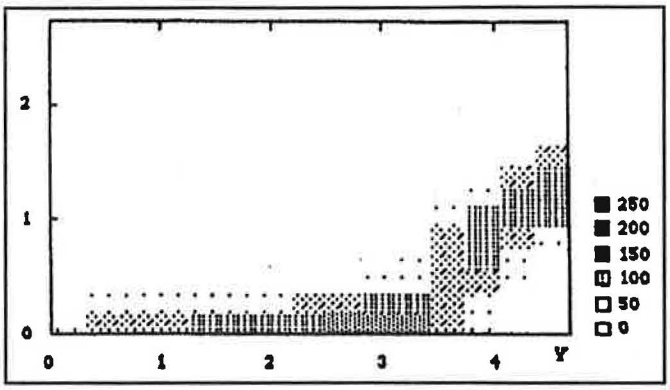
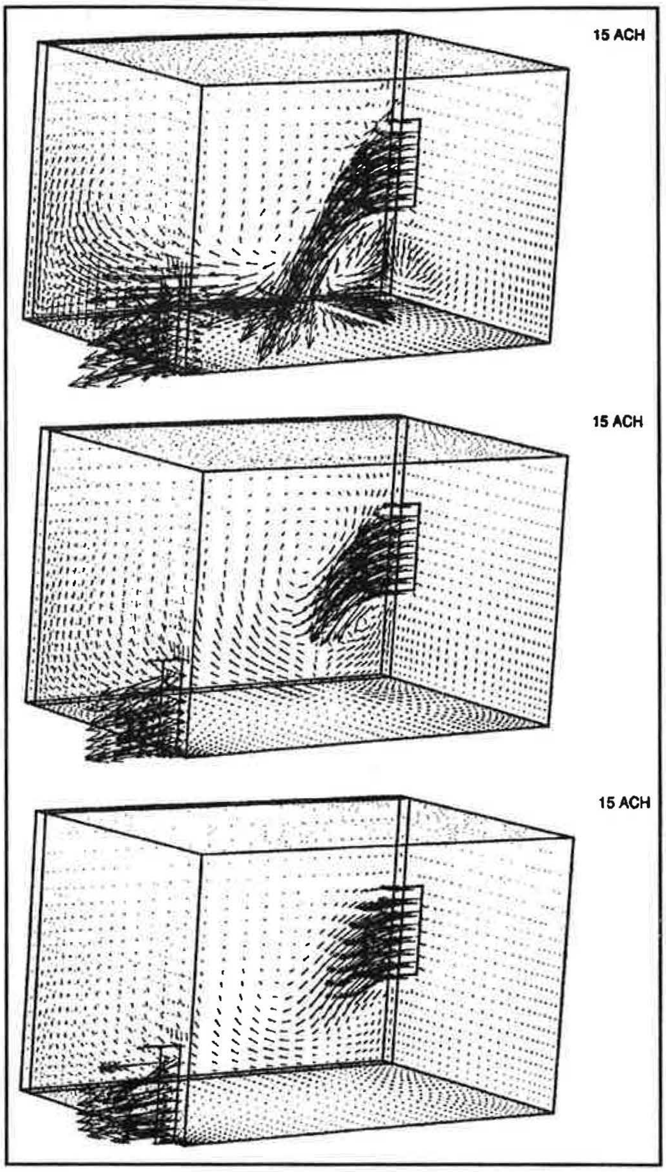


Figure 1b: The measured flow field speed distribution on the vertical plane in the room bisecting the supply duct. The "rastor graphic" data clearly confirm that the negatively buoyant supply jet descends sharply to the floor.



Figures 1c (top), 1d (middle) and 1e (bottom): The figures present the CFD simulation results for Re^t = 14, 29, and 149. The figures provide a 3-D perspective of velocity vectors on the mid-supply, room back wall and floor planes.

the very approximation process in CFD theory that leads to intrinsic error mechanisms that can range from benign to pathological. The ASHRAE professional who seeks to use CFD to assist in system design needs to be fully aware of these "two edges" of the "CFD sword."

How Good Can CFD Be?

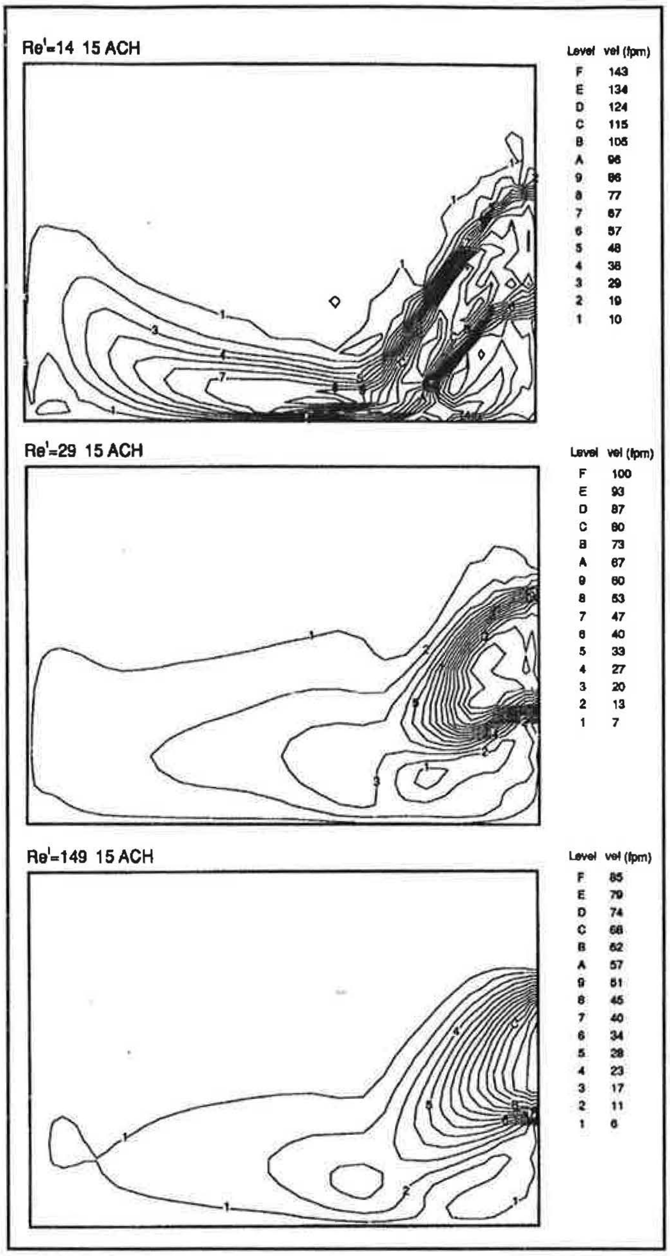
The fundamental question regarding CFD methodology, in application to room air motion prediction is, "Just how good is it, or can it be?" The companion concern must be, "what issues exist to compromise the ability of a CFD method to accurately simulate a given room air motion situation?" The underlying precept in seeking the answers is that, since all CFD procedures constitute the summation of a *significant* number of *assumptions*, it is unreasonable to expect the results of *any given* CFD simulation to be exact unless the problem definition is trivial, or great care has been exercised in design and execution of a set of CFD experiments.

CFD simulation may indeed be considered a new experimental protocol, parallel to the traditional physical laboratory experiment. In the "real laboratory," a carefully constructed scale model is tested using measuring devices specifically selected to control error during the data acquisition process. A CFD simulation experiment is analogously conducted in the "CFD laboratory," via a mathematical model running on a computer, with careful attention to sources of error that may compromise the (predicted) data.

The analytical (calculus) expressions describing the basic space-time relationships between mass, velocity and temperature have been available for over a century. Most of us were introduced to these "conservation laws" in undergraduate engineering/physics studies. Expressed in partial differential equation (PDE) form, for fluids the description is generally called the "Navier-Stokes (NS) equations." This PDE system may be directly applied to description of laminar flow fields (only!), however, almost all room air flows are at least locally turbulent.

For predicting turbulent flow, a mathematical manipulation on the NS equations (called *Reynolds-averaging*) is required for computational tractability [6]. Resolution of this time-unsteady flow, into a mean velocity description, and fluctuations about the mean, requires several assumptions. This process invariably leads to definition of a turbulent (called "Reynolds") stress-strain constitutive form containing a turbulent "eddy viscosity" and usually denoted ν^t. The elementary form for this Reynolds stress expression appears similar to the well-known Stokes laminar viscosity constitutive law with molecular kinematic viscosity ν. However, for laminar flow the viscosity ν is a property of the fluid itself (and weakly dependent on temperature), whereas the turbulent eddy viscosity ν^t depends on the state of the flow, hence varies widely over the flow field.

Therefore, a principal assumption for a CFD simulation is the turbulence closure model for the governing Reynolds-averaged Navier-Stokes (RaNS) partial differential equation system. The "standard" CFD selection has universally been the two-equation turbulent kinetic energy (TKE) model [6, 7], which adds two very non-linear PDEs to the RaNS set. To



Figures 1f (top), 1g (middle) and 1h (bottom): These figures present CFD data manipulated to speed contours on the supply duct mid-plane, for direct comparison to Figure 1b.

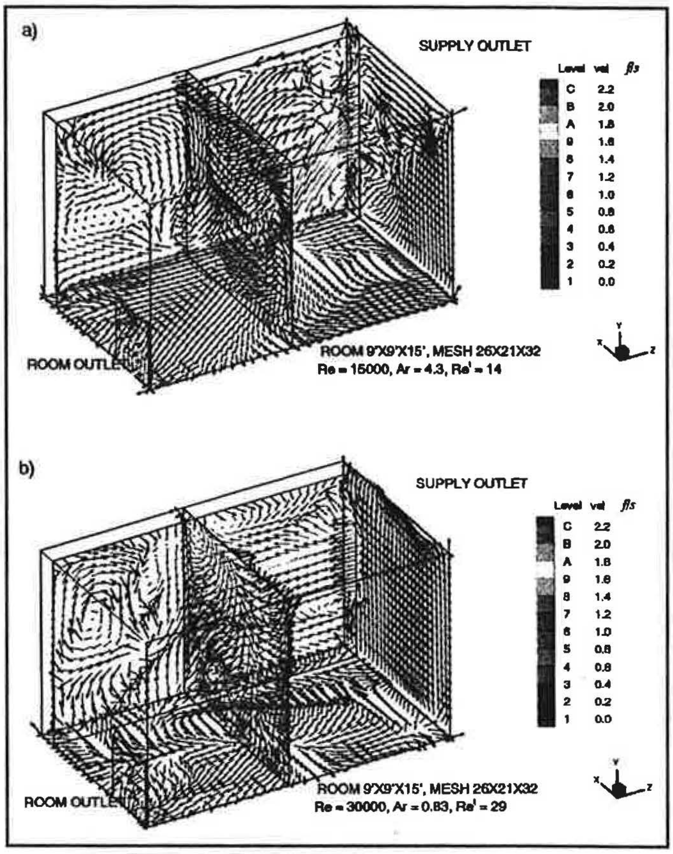


Figure 2: Figure 2a (top) presents CFD velocity vector distributions colored by speed on select cutting planes in the Spittler room at ACH=15. Figure 2b (bottom) presents the CFD experiment prediction for ACH=30.

within detailed decisions on boundary conditions, the TKE-RaNS selection yields a mathematically well-posed and computationally tractable system for CFD.

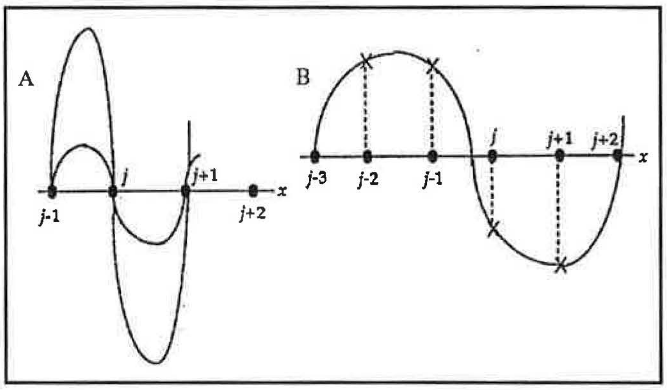
However, a *significant flaw* in the TKE model for room air applications is that it assumes a *fully turbulent flow* exists everywhere. In truth, at reasonable ventilation rates, the flow in full-scale rooms is likely to be fully turbulent only in supply ducts, near-by HVAC outlets, and downstream of the edges of obstacles. Elsewhere, the flow is more likely to be weakly-turbulent and genuinely time-unsteady, with a wide range of large-to-small scale flow structures. Therein, the TKE model will over predict the turbulent viscosity level, hence locally *add false diffusion* into the flow field CFD prediction.

TKE modifications for low turbulence applications have focused primarily on near-the-wall model adjustments. Generally speaking, such low-turbulence models have not been verified for CFD application to the field away from the walls and supply jets. A quantitative engineering measure of the degree of turbulence in a flowfield, and its simulation, is the turbulence Reynolds number (Re^t). It is defined as the ratio of the turbulence and kinematic viscosities, i.e.,

$$Re^t = \nu^t/\nu \geq 0$$

For a laminar flow, by definition the turbulence level is zero, hence $Re^t = 0$. The transition to turbulent flow occurs roughly in the range $5 < Re^t < 30$, and for fully turbulent flows $50 < Re^t < 10^3$. Of course, any genuine room flow will exhibit a large range of Re^t.

Thus, the answer to the question "How good can CFD be?" is very dependent on the form of the RaNS PDE selected and the boundary conditions. Errors which result from poor selections are not easy to assess until more comprehensive forms of turbulent flow PDEs are derived and validated. Therefore, since no CFD room air simulation can be exact, a range of CFD simulations, i.e., "*CFD experiments*" must be conducted to verify solution sensitivity to closure model parameters and boundary conditions embedded in the selected RaNS system, and their numerical implementation.



Figures 3a (left) and 3b (right): A CFD mesh is incapable of "resolving" any solution information with a wavelength of two cell widths or less. As illustrated in Figure 3a), since the nodal values of the 2 Δx sine wave are all zero, the mesh obviously cannot resolve that this wave exists. Conversely, significantly longer (e.g., 5 Δx) wavelength data are quite well observed on the nodes of the mesh, Figure 3b).

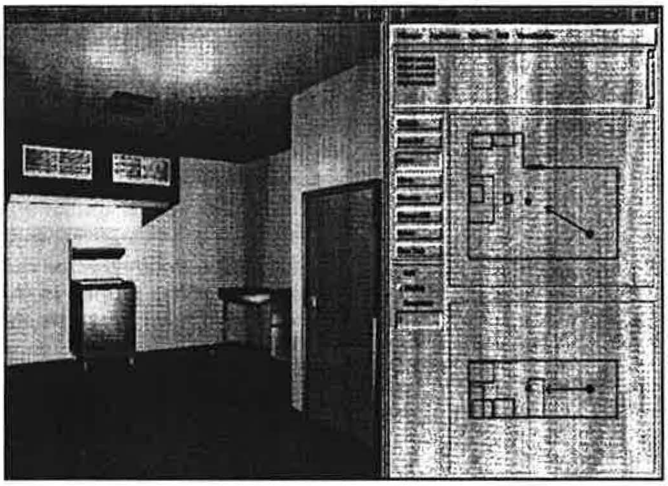


Figure 5: This figure illustrates the windows view the designer of a commercial kitchen might see when selecting disposition of equipment and the HVAC supply/ exhaust

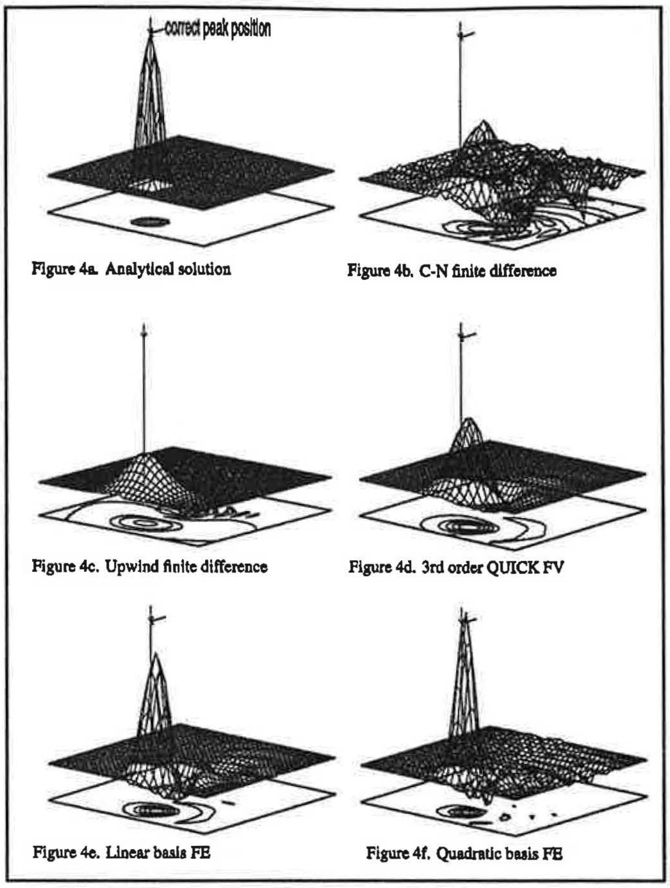


Figure 4: Control of artificial diffusion is a critical issue for accurately simulating room air motion. It is a good idea to run test cases with known solutions, which are called verifications.

Conducting CFD Experiments

The *quantitative* diagnostic utility of "CFD experiments" is reported in [3] for the buoyant mixed-convection full-scale empty room experiment of Spittler [8]. Select flow field magnitude (speed) and temperature data were measured and reported for several settings in a full-scale ventilation test facility, for air exchange rates ranging $15 \le ACH \le 100$. Employed wall heating panels, and the room ceiling and floor were insulated. The ventilation system supplied cold air, $T_s = 20°C$ (69.8°F), to the initially hot room with heated walls, $T_w = 27°C$ (83°F), via an open, mid-height end-wall supply duct. The room exhaust was at floor level, kitty-corner to the supply, as illustrated in *Figure 1a* scaled by a "graduate student." The test Archimedes number (Ar) was 4.3 and the Reynolds number (Re) was 15,000. Recall that Re scales convection to diffusion level, while Ar scales thermal buoyancy effect to Re squared.

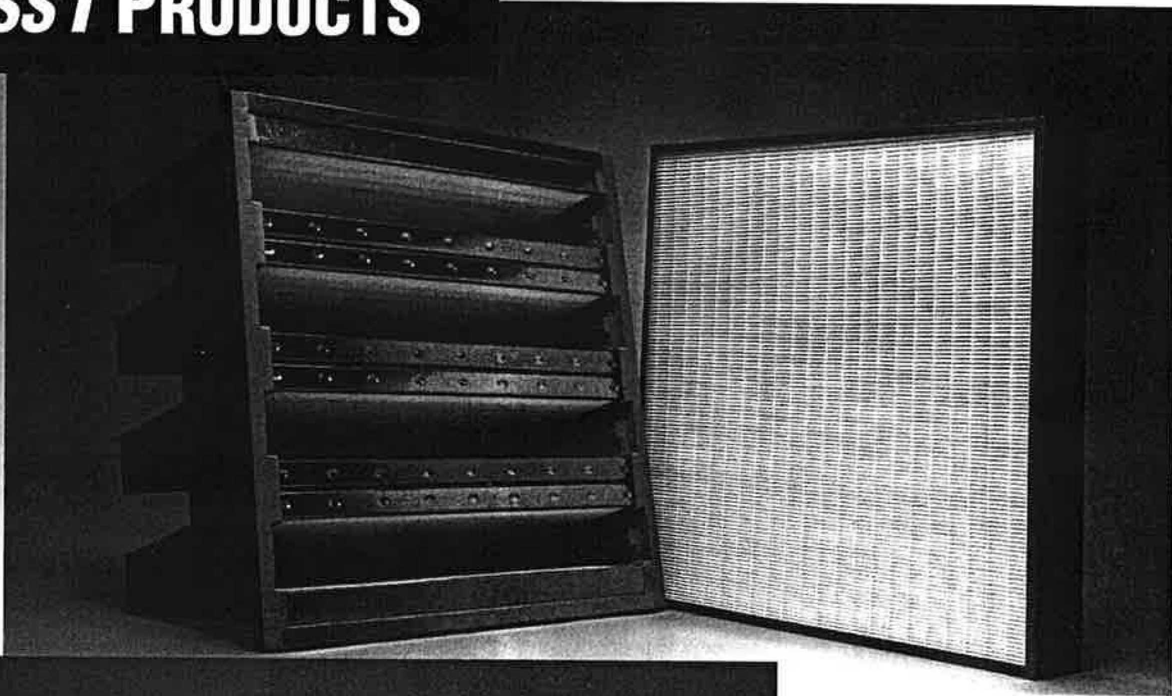
For the large, vaneless supply opening, the 3-D room airflow field was anticipated to be "low" turbulence level, an assumption requiring verification by conducting "CFD experiments." Following some tests on CFD meshing requirement [3], a nominal 20,000 element meshing with domain discretization extensions into both the room supply and exhaust ducts (for consistent boundary condition application) was selected. For the experiments, the base (laminar) flow diffusion/convection level is characterized by inverse Reynolds number, Re^{-1}, which was then augmented by $Re^t > 0$ over a select range. The net result is a CFD-defined balance between fluid (convection) and modeled diffusion processes in the form

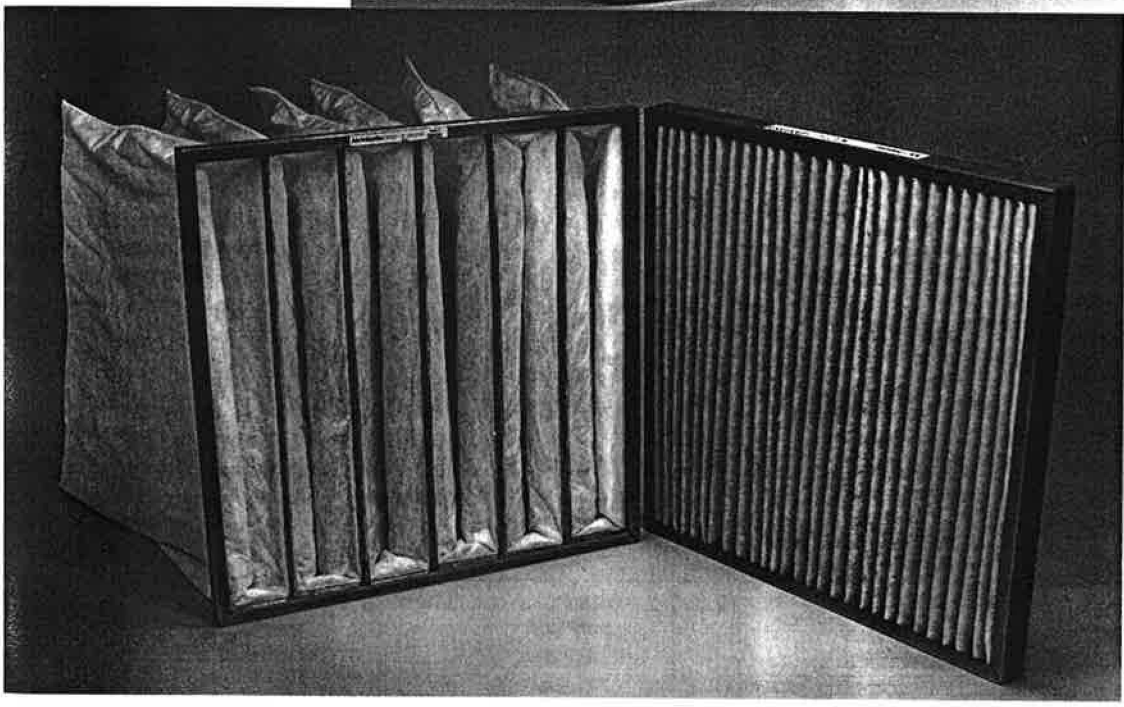
$$\frac{\textit{diffusion processes}}{\textit{convection}} \approx \frac{1}{Re}[1 + Re^t] \ll 1$$

Hence, for the low-turbulence setting $Re^t = 14$, for example, the simulation diffusion level is 15 times larger than laminar, i.e., $[1 + 14]/15{,}000 = 10^{-3}$, hence the diffusion level scales at only one *one-thousandth* of convection! The higher "low" turbulence CFD setting of $Re^t = 29$ changes the proportion to 1/500, while the "fully" turbulent level of $Re^t = 149$ produces a 10^{-2} diffusion/convection ratio.

Figure 1a) presents a scale perspective of the room, showing supply and exhaust duct locations. *Figure 1b)* graphs the measured flow field *speed* distribution [8] on the vertical plane in the room bisecting the supply duct. These "rastor graphic"

See CFD, Page 56





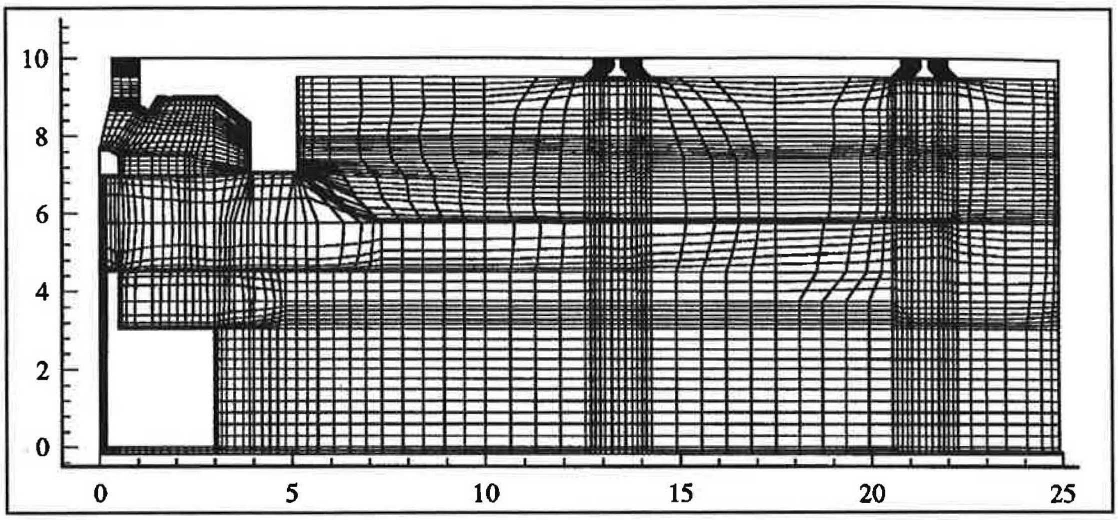


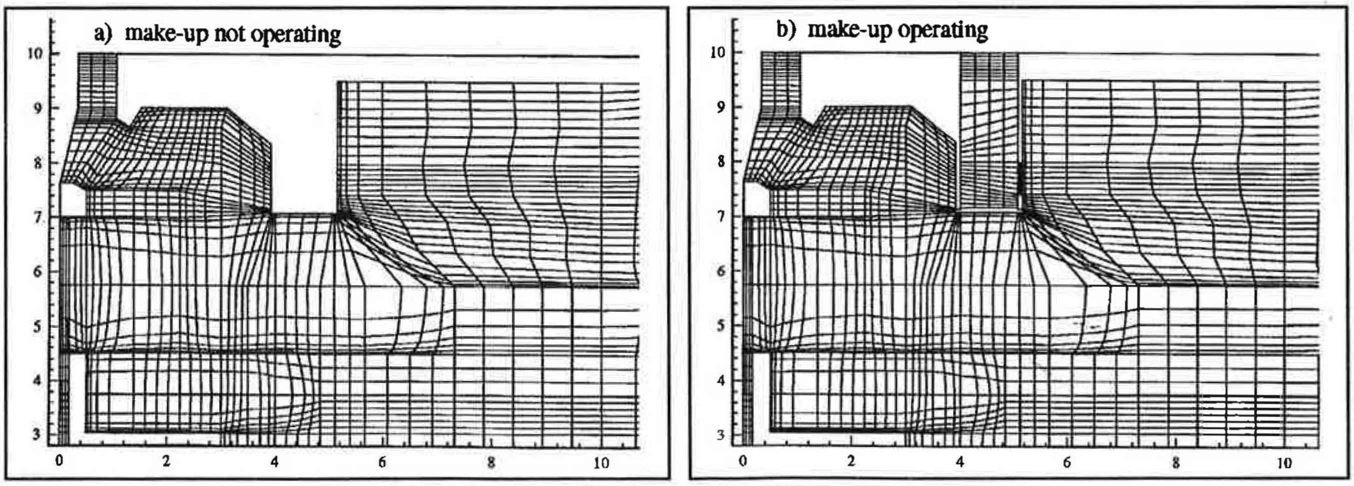
Figure 6: The CFD meshing end result for a symmetry centerplane slice of a full-scale facility measuring 25 ft. (7.5 m) in length with a 12 ft. (3.6 m) ceiling height.

CFD, From Page 54

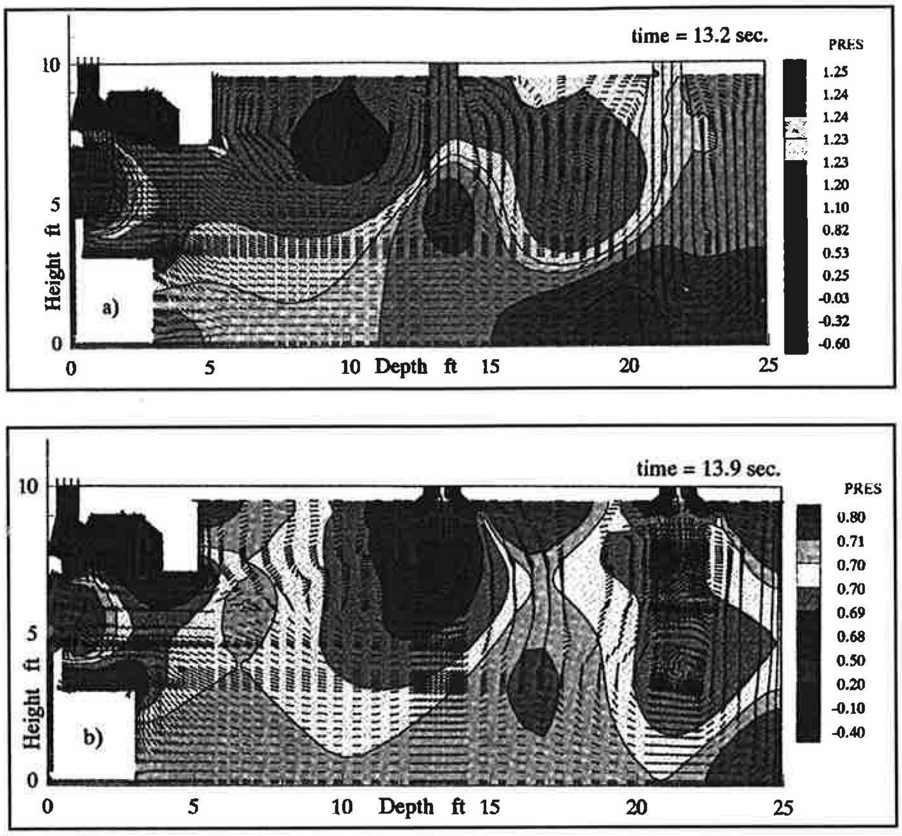
data clearly confirm that the negatively buoyant supply jet descends sharply to the floor, hence proceeds across it with negligible vertical diffusion, eventually decelerating as it approaches the exhaust plane wall. *Figures 1c), 1d), 1e)* present the CFD simulation results for $Re' = 14$, 29, and 149, as a 3-D perspective of velocity vectors on the mid-supply, room back wall and floor planes. *Figures 1f), 1g), 1h)* present these data manipulated to speed contours on the supply duct mid-plane, for direct comparison to *Figure 1b*.

Clearly from these CFD experiments, the simulation result agreeing best with the available test data occurs for $Re' = 14$. For the other two settings, the jet never hits the floor, due only to the *excessive diffusion* associated with the turbulence-level definitions $Re' = 29$ and 149. These CFD experiment data thus confirm the room flow is low turbulence level as originally anticipated. Importantly, it is graphically evident that excess modeled-turbulent diffusion can thoroughly compromise a CFD prediction for low-turbulence level room airflows. Exerting control on *modeled turbulence effects* is thus central to accurate room air motion CFD simulation, which should result with establishment of more appropriate turbulence models, cf. [9].

CFD simulation offers a heretofore unavailable interpretation of "what goes on" with supply jet introduction into a three-dimensional room. One tends to think "unidirectionally," i.e., the supply flow simply turns towards the room exhaust and leaves. This is far from the truth, as amply illustrated in *Figure 2a*, presenting velocity vector distributions colored by speed on select cutting planes in the Spittler room. Note the supply jet *accelerates* by a factor of two in dropping to the floor, as a multitude of recirculating flow regions are induced in the "turning process" towards the exhaust. Hence, the 3-D room flow is far from unidirectional. An experiment was conducted [8] for doubling of the supply jet velocity, hence Re=30,000 and the negative buoyancy effect was decreased by a factor of about four to $Ar = 0.83$. *Figure 2b* presents the CFD experiment prediction, as select planar velocity vectors colored by speed. For this flow specification, these data confirm creation of a room-scale, S-shaped vortex mid-way into the room, as the manner in which the supply flow reaches the exhaust. Interestingly, this prediction is verified by CFD experiments to be essentially *insensitive* to modeled turbulence level [4], over the same range as for the $Ar = 4.3$ simulations.



Figures 7a and 7b: The local finite element meshing options for a canopy hood. This CAD-generated basic discretization is amenable to on-screen interactive constructions.



Figures 8a (top) and 8b (bottom): Figure 8 presents the computed symmetry-plane velocity vector field distribution at steady state, superimposed on the computed pressure distribution (with discrimination in hundredths of inches of water). In Figure 8a, simply dumping the supply air into the kitchen produces jets that penetrate vertically to near floor level, hence turn towards the appliance and out the canopy hood exhaust. Conversely, Figure 8b summarizes the companion CFD simulation, where the supply is exhausted via 45° dual-slot diffusers

The Basic CFD Error Mechanism

Controlling strictly numerical *artificial diffusion effects* is also critical to conducting *quality* CFD experiments. An engineer looking to simulate room air motion can call upon many CFD theories (and codes), e.g., finite difference, finite volume, finite element. But each share the liability that they can generate *only an approximation* to the genuine solution of the selected RaNS PDE system. One basic reason that true solutions cannot be attained via CFD is that computational theories employ a *discretization* or "computational mesh" to support the numerical process. The solution comes out as *numbers* at the intersection loci (nodes) of this mesh, and they must be sufficiently dense to resolve, i.e., be "able to see," the essential (spectral) content of the flow field.

Fundamentally, a CFD mesh is incapable of "resolving" any solution information with a wavelength of two cell widths or less. As illustrated in *Figure 3a)*, since the nodal values of the 2 Δx sine wave are *all zero*, the mesh obviously cannot resolve that this wave exists. Conversely, significantly longer (e.g., 5 Δx) wavelength data are quite well observed on the nodes of the mesh, *Figure 2b)*. The obvious conclusion is that "an adequate mesh is an inescapable requirement" in CFD!

This mesh resolution issue is absolutely fundamental; if flow data are unresolved by the mesh, computational results cascade to longer wavelengths which show up as mesh-scale oscillations, i.e., "wiggles," when the solution is plotted. (Algorithm node-to-node decoupling can also produce mesh scale wiggles.) This oscillatory error mode can produce unrealistic results, such as negative contaminant concentrations, or may actually cause divergence of the CFD algorithm non-linear iteration process. This is a very undesirable result, so CFD theory/code designers have developed numerical diffusion methods to *dissipate the oscillations* by strictly artificial means.

The use of "sufficiently fine" meshes in a genuine 3-D large scale room simulation is computationally impractical unless a supercomputer is available. Hence, the universal CFD cure to oscillations is to add *artificial viscosity* (ν^a) to introduce strictly numerical dissipation, a diffusive mechanism which adds to that produced by the physical (ν) and modeled turbulent diffusion (ν^t) processes. Without close attention to detail, such artificial diffusion mechanisms can totally dominate the real processes, hence corrupt the solution.

Control of artificial diffusion is a most critical issue for accurately simulating room air motion. It's a good idea to run test cases with known solutions (called *verifications*), to make sure this error mechanism is under known control. For room contaminant transport, a classic definitive verification problem is pure convection of a gaussian-shaped puff of contaminant in a solid-body vortex velocity field, the so-called "rotating cone" test case. *Figure 4a)* presents a perspective view of the initial concentration distribution and the sense of flow rotation is clockwise. Since no physical diffusion is specified, this is also the graph of the *exact solution* after any number of complete circulations of the gaussian puff around the *x-y* plane.

Figure 4b) presents the base Crank-Nicolson finite difference solution after one circulation; the mesh unresolved short-wave error cascade to longer wavelengths is very graphic. The use of a simple algorithm upwind convection form induces an artificial diffusion mechanism producing unacceptable loss of the peak, *Figure 4c)*, although the error oscillations are certainly contained! Most commercial codes today replace upwinding with a "QUICK" convective upwind-differencing scheme, and

Figure 4d) confirms the substantial improvement but unacceptable accuracy. The Galerkin finite element method is mathematically superior to either of these "corrections," [7], and *Figures 4e-4f)* confirm significantly better peak retention with relatively smaller trailing wake oscillations. Note however, that even these "better" solutions exhibit dispersive error, the unavoidable price of "approximation" using today's CFD theories.

Designing with CFD

To date, essentially every CFD room air motion paper in the literature presents flowfield prediction in an empty room devoid of HVAC supply ducts, diffusers, furniture and people. This leads to questions about the value of this methodology if the very entities that facilitate design are absent from the CFD simulation. It's obvious that design functionalities must be brought into the CFD simulation capability.

Moving CFD to the *design arena* requires the integration of CAD for definition of geometry and entities in the practical room environment. *Figure 5* illustrates the *windows* view the designer of a commercial kitchen configuration [10] might see for selecting disposition of equipment and the HVAC supply/exhaust system. The CAD library contains placeable entities, e.g., cook-top fryers, ovens, deep fryers, canopy and makeup air hoods, etc., as well as HVAC system supply diffusers. They are brought to an initially empty room by mouse click-and-drag operations, such that a commercial kitchen can be completely configured for CFD simulation of a potential orientation of equipment and ventilation.

The key CFD attribute of this developing "kitchen.VIEW" system is that once defined, one moves directly into the mesh generation and discretization phase for a CFD prediction of probable flowfields, as a function of supply balance and diffuser selection. *Figure 6* illustrates the end result for a symmetry centerplane slice of a full scale facility [10], measuring 25 ft (7.5 m) in length with a 12 ft (3.6 m) ceiling height. For CFD assessment, this slice contains a cooktop fryer, a canopy make-up air hood and 2 HVAC supply slot diffusers with variable vane angle.

Of particular note is the above-ceiling supply duct geometric detail, included to admit various diffuser geometries via meshing into the supply ducts where remote (known) boundary conditions can be applied. This CAD-generated basic discretization is amenable to on-screen interactive constructions of locally refined grids, as well as the option for including flow prediction within and downstream the makeup air plenum of the canopy hood, *Figure 7a-b*.

The fundamental impact that HVAC slot diffuser selection has on the CFD-predicted symmetry plane flowfield is easily illustrated. *Figure 8* presents the computed symmetry-plane velocity vector field distribution at steady state, superimposed on the computed pressure distribution (with discrimination in *hundredths* of inches of water). In *Figure 8a*, simply dumping the supply air into

It is extremely important that ASHRAE professionals seeking to use CFD gain a firm understanding of its limitations and shortfalls, such that confidence can be assured that the numerous error mechanisms intrinsic to CFD are not compromising the predicted results.

the kitchen produces jets that penetrate vertically to near floor level, hence turn towards the appliance and out the canopy hood exhaust. Recirculation regions are created in the upper half of the kitchen, with ample evidence of the (non-symmetric) entrainment action caused by the supply jets.

Conversely, *Figure 8b* summarizes the companion CFD simulation, where the supply is exhausted via 45° dual -slot diffusers. Note that the main kitchen flowfield character is *entirely opposite* (!) from the previous case, although it still ends up leaving via the canopy hood exhaust. In particular, looking directly underneath the supply diffuser, note that room air is flowing *up* to the ceiling, rather than directed away for the simple dump diffuser. One may recall the observation that "dirty" ceiling diffusers indicate good circulation.

Summary

In preparing this article, the authors have bounded their enthusiasm for the bright prospects that CFD brings to the HVAC industry with dashes of reality. It is extremely important that ASHRAE professionals seeking to use CFD gain a firm understanding of its limitations and shortfalls, such that confidence can be assured that the numerous error mechanisms intrinsic to CFD are not compromising the predicted results. Carefully executed CFD experiments can definitely help the HVAC system designer gain a better understanding of the intricacies of probable flow patterns for the choice of diffusers and room obstacles.

Confidence in such CFD predictions is gained only after the methodology has been proven via computing pertinent verification and benchmark problems. Quality CFD methods can predict very low-level velocity fields, and subtle pressure variations, where experimental apparatus has great difficulty. Therefore, except in the immediate vicinity of a supply diffuser where large velocities can be measured, validation of CFD predictions must by and large come from conducting a *range* of *quality* CFD experiments on the design options for a configuration. A single CFD prediction is and will remain to be essentially valueless.

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