

WIND TUNNEL AND NUMERICAL SIMULATION OF POLLUTION DISPERSION: A Hybrid Approach

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ABSTRACT: This review will examine the application of fluid and numerical modeling to air pollution aerodynamics. Air pollution aerodynamics concerns the interaction of noxious aerosols, gases and particles emitted into the atmosphere with surrounding structures, terrain and vegetation. This interaction can deflect materials toward sensitive areas, concentrate species above acceptable levels, or even mitigate concentration levels and enhance diffusion and dispersion.

1 INTRODUCTION

There is a renewed interest in dispersion modeling due to the need for tools that can be used for responding to, planning for and assessing the consequences of releases of gases, aerosols and particles from industrial, transportation, and even terrorist activities. Such release configurations are often too complicated to predict reliably by the host of analytic models developed primarily for evaluating the long-term (annual or seasonal) effects of pollutants in limited and idealized situations¹. A reliable new *hybrid* methodology has arisen that combines the advantages of an old tool, fluid (physical or scale) modeling, with the speed and convenience of a new technology, computational fluid dynamics (CFD). The traditional view is that the scientific method has two foundations; experimental and theoretical (Figure 1). While the traditional scientific method does not acknowledge the role for computing and simulation, a new paradigm establishes a foundation for the extension of the traditional processes to include verification and scientific software development. This framework elucidates the relationships between the processes of scientific model development, computational model verification, and simulation validation (Figure 2). For example, fluid modeling can initially provide data from which CFD turbulence models are created, CFD calculations can use such turbulence models to quickly survey alternate solution strategies using simplified domain scenarios, then physical modeling can examine in greater depth design consequences, and finally, CFD can extend initial conclusions to a broader

¹E.g. U.S. EPA Support Center for Regulatory Air Models or SCRAM, <http://www.epa.gov/scram001/tt22.htm#rec>.

set of similar cases. Combining experiments with numerical simulations also provides new educational opportunities for the next generation of engineers and scientists (Guessous et al., 2004).

1.1 *Fluid Modeling*

Wind or water tunnels are, in effect, analog computers that have the advantage of “near-infinitesimal” resolution and “near-infinite memory.” A fluid modeling study employs “real fluids” not models of fluids; hence, the fluid model is implicitly non-hydrostatic, turbulent, includes variable fluid properties, non-slip boundary conditions, and dissipation. Real fluids permit flow separation and recirculation. All conservation equations are automatically included in their correct form without truncation or differencing errors, and there are no missing terms or approximations. The basic equations of motion and transport are solved by simulating the flow at a reduced scale, and then the desired quantity is measured. Finally, the fluid model bridges the gap between the fluid mechanician’s analytic or numeric models of turbulence and dispersion, and their application in the field. Fluid modeling may be used to plan field experiments, provide conservative estimates of plume transport, and validate modules of numeric code (Snyder, 1981; Meroney, 1986a).

1.2 *Computational Modeling*

Numerical modeling, despite its many limitations associated with grid resolution, choice of turbulence model, or assignment of boundary conditions is not intrinsically limited by similitude or scale constraints. Thus, in principle, it should be possible to numerically simulate all aspects of plume transport, dispersion, and/or drift. In addition it should be possible to examine all interactions of plume properties individually, sequentially and combined to evaluate nonlinear effects (Murakami, 1999; Stathopoulos, 1999). It is this tremendous potential that has led wind engineering practitioners to more frequently present results of such numerical studies in professional and trade journals and promotional materials. Realistically, however, the choice of domain resolution, turbulence models, and boundary conditions constrain predictions. The tendency for many CFD users to believe implicitly in the realism of the beautiful graphical displays that their software produces is implied when one says that CFD is really an acronym for “*Colorful Fluid Dynamics*.” Harsher critics say that “*Cheats, Frauds and Deceivers*” would be more appropriate (Spalding, 1999).

Hence, continued verification and validation is required at almost every level of CFD prediction (Castro and Graham, 1999; Castro et al., 1999; Castro, 2003; Robins et al., 1998; Slater, 2004).² Various criteria for measuring agreement between predictions and full or model-scale measurements are available including scatter diagrams, classical ANOVA, pattern comparison tests and weighted average fractional bias plots (Shin et al., 1989, 1991). Several organizations have established committees and groups to focus on the quality of and trust in CFD applied to practical applications (E.g. QNET-CFD, 2004; NPARC Alliance, 2004; ERCOFTAC, 2000; AIAA, 1998). Meroney (2003, 2004b), Meroney et al. (2000, 2002a, 2002b, 2002c) and Banks et al. (2003) all validated their FLUENT calculations for a variety of bluff-body and urban street canyon configurations by comparing with measurements taken during physical model simulations. These comparisons revealed which situations were modeled with confidence, and which configurations produced less reliable predictions.

1.3 *Hybrid Modeling*

There are several reasons why joint fluid/computational modeling should be useful for evaluating the validity of dispersion models and even directly predicting the behavior of dispersion during diffusion incidents: theoretical, dispersion comparability, controlled conditions and expense.

The very use of the word “hybrid” implies a combination of initially unrelated concepts of heterogeneous origin that results in an offspring that has hopefully the best qualities of both parents. Indeed, such crossbreeding often results in ‘hybrid vigor’ that has even better and stronger characteristics than either parent. For example,

- Both methods permit the individual control of many variables which permits the analyst to isolate driving or dominant transport mechanisms,
- Fluid modeling can provide data in situations where the actual physical mixing mechanisms are vague, confused or obscured by other phenomena,
- Computational modeling can provide data at greater spatial resolution than is practicable during fluid modeling due to instrumentation, time or cost limitations, and/or

²*Verification* is defined as the process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model. Qr: Procedure to ensure that the program solves the equations correctly. *Validation* is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Qr: Procedure to test the extent to which the model accurately represents reality.

- Dispersion in fluid modeling situations incorporate mixing at all time scales, whereas time dependent solutions in CFD often require the dedication of massive computational resources.
- Computational modeling can be employed to explore further into the parametric space of a problem.

When used together the analyst is able to confidently assess model reliability, model generality, and model robustness. Indeed engineering groups are often reluctant to make critical design decisions based solely on CFD, instead acquiring similar data from independent sources, such as wind tunnel testing, that mitigates the perceived risks due to feared deficiencies in CFD data. Viegas remarked during the 1993 NATO Advanced Study Institute on Wind Climates in Cities that “numerical and experimental methods are complementary, the ideal situation being that both of them are carried out in parallel.” (Cermak et al., 1995)

In the following review sections Chapter 2.0 examines the chronological development of fluid modeling and numerical techniques as applied to air pollution aerodynamics. Chapter 3.0 describes the similitude concepts used in fluid modeling and reviews ten application areas of fluid modeling in air pollution aerodynamics including effects of stack exhaust momentum, plume buoyancy, building effects, atmospheric stratification, complex terrain, dense gases, natural ventilation, droplets and drift, fires, and urban building configurations. Chapter 4.0 elaborates on the concept of hybrid modeling using resources both from fluid modeling and numerical methods. The chapter provides several examples of hybrid modeling familiar to the author. Finally, Chapter 5.0 summarizes research needs identified by the author and suggests new research initiatives.

2.0 LANDMARKS IN AIR POLLUTION AERODYNAMICS

Many outstanding scientists have contributed to the growth of our understanding of Air Pollution Aerodynamics. Contributions have been recorded in many journals, reports, and proceedings. Many are in languages other than English and archived in limited locations. My presentation reflects my own experience, resources, preferences and memory. It was certainly not my intention to ignore or forget anyone’s contribution, but the limited scope of this review is evident. I trust every reader will find some value.

2.1 *Chronology of Applications of Fluid Modeling*

Among the earliest studies of plume behavior near buildings was that by Sherlock and Stalker (1940) who studied smoke plumes emitted from stacks above a model of the Crawford Power Station, Chicago Il. They combined their evidence of downwash with local climatological data to predict percent duration of downwash for different wind and stack exhaust velocities. Similarly, Hohenleiten and Wolf (1942) reported plume outlines for models depicting the Riverside Power Station, Baltimore, Md. They used their data to mitigate the possibility of plume interference with planes flying from a nearby airport.

The earliest quantitative wind tunnel diffusion study may have been that performed by McElroy et al (1944) who studied a chimney jet in a built-up area. They used two models constructed to scales of 1/200 and 1/400 to study concentrations expected within 150 m of a 12 m square, 77 m high chimney discharging contaminated exhaust air from the proposed Brooklyn-Battery tunnel. Values of emission velocities, V , and wind speeds, U , were varied to produce a range of ratios from 0.3 to 10. Isoleths of maximum concentration ratio ($C_{\text{local}}/C_{\text{source}}$) were found as well as discrete points on adjacent buildings. Authors found scale effects were absent, but no attempt was made to simulate the approach boundary layer.

During WW II studies were performed by Kalinske et al (1945a, b) or Rouse (1951) at the University of Iowa to study the dosage and maximum concentration at various locations in a Japanese urban area as a result of exposure to a wind-borne gas cloud which had been created by a bomb burst in the area. A 1/72-scale model of a typical area was installed on the floor of a 2 m wide x 6 m long x 1.3 m high wind tunnel. The maximum height building was 100 mm, but the buildings covered the entire tunnel floor. A pancake-shaped burst was produced by emitting gas through a graded set of holes in the floor. Wind speeds were about 3 m/s. SO_2 concentrations were measured horizontally and vertically among the downwind buildings and reported non-dimensionally as CL^2U/Q , where U was the reference velocity and L a reference length. Results were compared with field tests over a full-scale Japanese village at the Dugway Proving Ground, UT, USA. Phosgene and NO_2 gas-filled bombs were released at the field site, but test variability made comparisons with the wind tunnel results questionable. The authors concluded results were order-of-magnitude and qualitatively similar. Wind tunnel accuracy was at least as good as the accuracy of single field experiments.

Bryant (1949) and Bryant and Cowdrey (1955) studied transverse jets in low-turbulence wind tunnels. Like most early studies plume spreading and trajectories were determined visually

which led to difficulties in defining behavior far downstream. It was usually difficult to see differences between transitional and ultimate rise, especially if the plumes were buoyant.

Between 1945 and 1955 wind tunnel diffusion work in the USA was primarily active at the University of Michigan (Sherlock and Lesher, 1955) and at New York University (Strom and Halitsky, 1954). Most measurements involved photographic examination of smoke visualization above power station complexes.

In the late 50s and 60s fluid modeling studies were conducted in many countries. In the USA the principle efforts were at Colorado State University (CSU); University of Michigan (UM); and New York University (NYU). The first true Boundary Layer Wind Tunnel was conceived at CSU by Cermak and Albertson (1958) and installed in the Fluid Dynamics and Diffusion Laboratory. At CSU Cermak and coworkers studied point, line, area, and volume sources in a turbulent boundary layer as well as dispersion over buildings [e.g. Children's Hospital, Washington D.C.; Rancho Seco Nuclear Power Station, CA; Denver Center of Performing Arts, CO], complex terrain [e.g. Point Arguello, CA; San Bruno Mountain, CA; Elk Mountain, WY; Stringfellow Dump Site, Riverside, CA], coastal sites [Avon Lake Power Station, OH], valleys [Wolf Creek pass, CO; Colorado River, CO], islands [San Nicolas Island, CA], dispersion in vegetative canopies, infiltration into buildings, dispersion in stratified flows, dense gas dispersion, and dispersion in urban street canyons. At UM Martin (1965) investigated dispersion about a model nuclear reactor building and compared model data with field experiments. At NYU Strom and coworkers studied dispersion about prismatic and round building shapes [e.g. EBR-2 reactor complex at the National Reactor Test Station, ID; the National Institute of Health, Bethesda, MD.], dispersion in stratified flows, and dispersion in urban street canyons.

In Europe work began with the critical studies by Jensen and Frank (1963) in Denmark that identified the importance of surface roughness and boundary layer turbulence structure during fluid modeling of the atmosphere. They extended their model studies of wind shelter phenomena over scaled surface roughness (including one roughness due to a model city) to diffusion from isolated chimneys, diffusion from chimneys mounted above gable roof buildings, and the effect of chimney cross-section on plume behavior. They expressed concentration measurements non-dimensionally but as $Cz_0^2 u^*/Q$, where z_0 is the roughness height and u^* is the surface friction velocity.

The Fluid Modeling Facility was founded by the U.S. Environmental Protection Agency (EPA) in Raleigh, North Carolina, in the 1970's. At this facility Snyder and coworkers studied a variety of problems associated with dispersion over idealized building shapes, stratified flow over complex terrain [e.g. Rattlesnake Ridge, AZ; Cinder Cone Butte, ID], and stack plume behavior.

In England the contributions of Barrett and Hall at the Warren Springs Laboratory, Dept of Environment and the work by Castro and Robins at the Central Electric Generating Board Laboratories at Leatherhead and Southampton must be mentioned. These groups developed innovative measuring equipment (e.g. pulsed-hot wire anemometers, fast response gas chromatography) and improved boundary layer simulation methods (e.g. elliptic Counihan spires).

By the end of the 1970s the application of fluid modeling to air pollution aerodynamics problems had become routine in new facilities in almost every industrialized country in the world. Both conventional and creative new facilities were added to many universities and government laboratories. Specialized facilities included aerosol tunnels, rainfall facilities, fire and smoke tables, stratified wind and water tunnels to study convective boundary layer phenomena, snow tunnels, ventilation chambers, and fire and smoke test chambers. The birth of the computer age opened up the possibility of computer enhancement to data acquisition and interpretation (computer aided engineering, i.e. CAE) such that previously tedious or exotic methods could be applied to air pollution aerodynamics (e.g. particle image velocimetry, laser-induced fluorescence, computer activated traversing systems, automated chromatography, and, of course, computational fluid dynamics!).

2.2 *Chronology of Applications of Computational Fluid Dynamics*

Long before the inception of electronic computer systems attempts were made to solve atmospheric problems by discretization of the fluid domain and numerical methods. In 1922, Lewis Fry Richardson developed the first numerical weather prediction (NWP) system. His calculation techniques (division of space into grid cells and finite difference solutions of differential equations) were precursors to modern computational fluid dynamics. Instead of an electronic computer he proposed to organize a “weather factory” manned by 64,000 human computers working in an amphitheater and coordinated to calculate world weather on adding machines and slide rules.

Mikio Hino (1968) was among the first to attempt numerical and wind tunnel comparisons of plume dispersion over complex terrain. The model experiment was performed at a scale of 1:2500 in a 1.5 m x 3.0 m x 10m long open-circuit Eiffel type windtunnel. The surface of the model was covered with pebbles to maintain turbulence and the boundary layer, and turbulence grids were placed upwind. Wind profiles measured over the rugged terrain exhibited speedup, separation, and stagnation regions. The terrain displaced experimental plumes, and plume spread and surface concentrations roughly followed trends predicted by his numerical model.

Routine applications of CFD to industrial applications began during the late 1960s at Imperial College of Science and Technology, London, UK, with the use of early generalized application programs like TEACH and GENMIX and kappa-epsilon turbulence models to predict flow and heat and mass transfer behavior for interior flows in furnaces, engines, heat exchangers, etc. (Launder and Spalding, 1972). During the 1970-1980 period many researchers worked to predict flow about airfoils and bluff bodies using CFD, but applications of CFD to air pollution aerodynamics situations really began quite recently with predictions of boundary layer flow over surface mounted cubes and groups of buildings (Murakami and Mochida, 1988). The distribution of field and wind tunnel data for wind flow over a rectangular test building from the CSU/TTU Cooperative Program in Wind Engineering (1987-2001) provided an additional surge of activity since, finally, extensive and credible wind tunnel and field data were available to validate numerical models (Bienkiewicz, 1995; Mehta and Meroney, 1995). The first International Symposium on Computational Wind Engineering occurred at the University of Tokyo in 1992, followed by the second at Colorado State University in 1996, and the third at University of Birmingham in 2000. These meetings accelerated the interest in using CFD to solve wind-engineering problems. Today almost every major national or international meeting devotes sessions to computational wind engineering topics.

Applications have become so numerous that reviews on CWE come out almost monthly! Recent work of interest includes that of McAlpine and Ruby (2004) on dispersion in micro-environments and Michael Brown (2004) on the need for fast response modeling to respond to urban terrorist incidents.

3.0 SIMILITUDE AND FLUID MODELING CONCEPTS

The concept of similitude is basically simple. Two systems at different geometric scales will exhibit similitude if a one-to-one correspondence exists in space and time between fluid particle kinematics (locations, velocities, accelerations and rotations) caused by fluid particle dynamics (pressures, gravity, viscous forces, etc.), when properly scaled by characteristic scales of fluid properties, force, length and time. To achieve this similarity, however, is not trivial. The specification of dimensionless parameters that guarantee similarity has historically been the subject of much discussion and debate. (Snyder, 1972; Meroney, 1988; Meroney, 1990; Barrenblatt, 1994)

In the nineteenth century a number of workers (most notably Lord Rayleigh) commonly solved problems by direct use of the similarity principle with the intuitive identification of relevant force ratios. During the early twentieth century, the force ratio methods lost favor and were replaced almost entirely by dimensional analysis, as represented by the Buckingham Pi theorem. The most systematic and reliable method currently used to identify relevant scaling parameters is the “normalization” of the governing partial differential equations of motion. Normalization makes the equations and boundary conditions nondimensional in terms of scaling variables of standard magnitude (Kline, 1965).

Scientists who examine the equations of motion including continuity, momentum, energy and species relations identify at least eight important dimensionless groups:

$$\begin{aligned}
 Ro &= U_R / (L S_R) \text{ is the Rossby number,} \\
 Eu &= P_R / (D_R U_R^2) \text{ is the Euler number,} \\
 Re &= D_R U_R L / \nu_R \text{ is the Reynolds number,} \\
 Ri &= g_R L / (T_R U_R^2) \text{ is the Richardson number,} \\
 Pe &= D_R c_{pR} U_R L / k_R \text{ is the Peclet number,} \\
 Pr &= \nu_R c_{pR} / k_R \text{ is the Prandtl number,} \\
 Sc &= \nu_R / (D_R D_R) \text{ is the Schmidt number, and} \\
 Ec &= U_R^2 / (c_{pR} T_R) \text{ is the Eckert number,}
 \end{aligned}
 \tag{1}$$

where subscript R refers to some characteristic reference condition. “Exact” similarity requires equality of the nondimensional coefficients listed above for the physical model and the prototype

situations. If separate length scales are chosen for the different coordinate directions, additional parameters are generated (e.g. Meroney and Melbourne, 1992)

Furthermore, boundary conditions governing the flow domain of interest must also be similar for the model and prototype. Surface boundary conditions would require similarity of topographical relief, surface roughness distributions, surface temperature distributions, and reproduction of associated obstacles, buildings, fences, source areas, etc. Similarity of the approach-flow characteristics requires similarity of distributions of mean and turbulent velocities, distributions of mean and fluctuating temperatures and humidity, and distributions of turbulent scales and energies. Similarity of the boundary conditions aloft would require similarity of the location of the upper streamline and near zero longitudinal pressure gradients.

The stipulation of some seven equations and boundary conditions, which contain some seven unknowns, U , V , W , T , p , D and P , indicate (in principle) their solutions can be determined. Any prototype and model flow that is constrained by the same scaled initial and boundary conditions, and for which all the dimensionless coefficients identified above are invariant, must have a unique solution in terms of the dimensionless variables. It is not necessary to actually solve the differential equations if one uses a laboratory facility as an analog computer. If all the foregoing requirements could be met simultaneously, then all scales of motion ranging from micro to mesoscale, i.e. 10^{-3} to 10^3 m, could be simulated within the modeled flow field.

Unfortunately, all similarity requirements cannot be satisfied simultaneously and modelers must use partial or approximate similitude. Hence model conditions must be chosen which are designed to simulate most accurately those scales of motion that are of greatest significance for the application (Cermak, 1974). Fortunately, several of the dimensionless parameters can be neglected due to their low relative importance when simulating transport and dispersion about buildings. For example, the Rossby number, which reflects the inertial effects of transport in a rotating coordinate system (the Earth), has minor influence unless motions persist over distances long enough for the associated spatial deviations to become significant. The Euler number is automatically simulated in air filled wind tunnels; the Richardson number may be neglected when atmospheric stratification effects are small or pertinent plumes are neutrally buoyant; the model and field values of Prandtl and Schmidt numbers for wind tunnel modeling of atmospheric flows are very close; and the Eckert number is generally small compared to unity for subsonic flows.

The magnitude of the Reynolds number indicates the relative importance of inertial forces and viscous or frictional forces. It imposes very strong limitations on rigorous simulation, since scale reductions of 1:100 to 1:1000 commonly result in model Reynolds numbers two to three orders of magnitude smaller than those found in the atmosphere. Thus the viscous forces are relatively more important in the model than in the prototype. If strict Reynolds number equality is required, no atmospheric phenomena could be modeled. Various arguments have been proposed to justify the use of smaller Reynolds numbers in model studies. Snyder (1972) reviewed suggested concepts of the laminar flow analogy, dissipation scaling, and Reynolds number independence. He concluded that only Reynolds number independence is a viable scaling possibility.

The thermal or mass species Peclet numbers can also be expressed as the product of a Reynolds number and the Prandtl number or the Schmidt number, ie. $RePr$ or $ReSc$. The parameter is a measure of the ability of the fluid to advect heat or mass compared with its ability to disperse heat or mass by molecular transport. The Peclet numbers become important when Reynolds number independence does not exist (Meroney, 1986a, 1986b, 1988).

Reynolds Number Independence Fortunately, it is possible to circumvent the effect of Reynolds number equality in many cases. Townsend (1956) suggested that, for a flow system in which thermal and Coriolis effects were absent and whose boundary conditions were similar when normalized by the appropriate characteristic length L and velocity U_R , the turbulent flow structure would be similar at all sufficiently high Reynolds numbers. Townsend called this hypothesis of Reynolds number independence “Reynolds number similarity.” Exceptions must be (a) the very small scale turbulent structures involved in the dissipation of turbulence into heat and (b) flow fields very close to boundary surfaces where the no-slip boundary conditions result in locally very small Reynolds numbers. Consequently, viscosity has very little effect on the bulk of the fluid motions.

But how does such similarity come about in the face of orders of magnitude of Reynolds number inequality? First, for simple flat plate and pipe flow situations it has long been observed that the surface drag coefficient which reflects momentum mixing rates becomes invariant with respect to Reynolds number when the surface is “sufficiently rough” and “sufficiently long”. Since the surface friction coefficient is invariant, the normalized mean velocity profiles that advect and shear plumes will also be invariant.

Second, the gross structure of the turbulence can be geometrically similar over a very wide range of Reynolds numbers. Consequently, flow-mixing rates will be similar when unmatched turbulent scales do not contribute significantly to dilution. Since in air pollution aerodynamics we often limit our observations to flow and dispersion near buildings and structures, we need not consider mixing induced by very large scales associated with plume meandering, weather or the diurnal cycle. It is the smaller scales of motion below the Van der Hoven spectral gap that are simulated in fluid modeling facilities. Thus, the equivalent upper limit for averaging time in laboratory facilities must be about 10 to 20 minutes.

Consideration of turbulent spectral plots show that a reduced Reynolds number changes only the higher frequency portion of a Eulerian spectral energy distribution. To determine whether such deviation from field scale behavior is critical, one must consider the contribution of individual scales to dispersion. Examination of the Taylor diffusion equation reveals that at very small travel times all scales of turbulence contribute to dispersion with the same weight, but for longer and intermediate travel times the larger scales of turbulence progressively dominate the dispersion process. Thus, eddies with scales less than one-tenth of the plume diameter or depth do not contribute significantly to the spread of the plume. If the fluid model replicates all eddy scales down to a small fraction of the building dimension, then one expects realistic plume dispersion a short distance away from a finite dimension source.

Previous Modeling Experience The most convincing evidence for the presence of adequate Reynolds number magnitude is obtained when laboratory evidence over a range of Reynolds numbers show that no strong deviations in concentration decay rate or plume growth occur. A number of authors have discussed flow studies about simple cubical or rectangular sharp-edged obstacles. Hosker (1984) provided an extensive review about such flow fields and the subsequent character of diffusion near obstacles. Unfortunately, though data for many fluid-modeling studies exist in the literature, few experiments have focused on the limiting role of the Reynolds number on transport and dispersion near buildings. Fluid modeling of atmospheric scale flows in wind tunnels requires the presumption that fluid motions, loads and mixing rates are independent of the ratio of inertial to viscous forces characterized by the Reynolds number, $Re = UH/\nu$. Such Reynolds number independence has been identified as a precondition for realistic simulation of transport and dispersion about buildings.

Golden (1961) measured the concentration patterns above the roof of model cubes in a wind tunnel. Two sizes of cubes were used to vary the Reynolds number from 1,000 to 94,000. The concentration isopleth in the fluid above the cube roof showed only slight variations over the entire range of Reynolds numbers studied. The maximum concentration on the roof itself was found to vary strongly with Reynolds numbers less than 11,000, but to be invariant with Reynolds numbers between 11,000 and 94,000. Frequently modelers quote Golden's experiments as justification for presuming dispersion invariance when obstacle Reynolds numbers exceeds 11,000. However, Golden's "11,000 rule" is limited to the measurement of concentrations at only one point on the roof of smooth-walled cubes placed in an uniform approach flow of very low turbulent intensity. Halitsky (1968) observed that for dispersion in the wake region no change in isoconcentration isopleth from passive gas releases was found to occur for values of Reynolds number as low as 3,000.

Castro and Robins (1977) performed an experimental investigation of the flow around surface-mounted cubes in uniform and irrotational versus sheared and turbulent flow conditions. Measurements of body surface pressures and mean and fluctuating velocities within the obstacle wake were made with pressure transducers and pulsed-wire anemometry. In the case of the uniform upstream flow and a cube normal to the flow, no changes in the flow field occurred beyond a cube Reynolds number of about 30,000. For a cube at 45° to the approach flow the high negative pressure measured near the top leading corner increased in magnitude by a factor of three as the Reynolds number increased from 20,000 to 100,000, which might suggest a very high critical Reynolds number for this situation. For the case of a turbulent upstream boundary-layer flow, no Reynolds number effects were discernible for situations corresponding to a Reynolds number based on cube height and the velocity at that height in the undisturbed flow of about 4,000.

Fackrell and Pearce (1981) examined wind tunnel measurements of near-wake parameters for many different building shapes in a variety of boundary layer flows. Measurements of recirculation region (cavity) characteristics at Reynolds numbers of 5,000 and upward showed no significant differences in residence time or recirculation region length. They concluded their results were independent of Reynolds number.

Parallel studies of the effects of Reynolds number on plume dispersion near cubes oriented normal to the flow field were performed in a water drag tank and a boundary layer wind tunnel by Snyder (1992). All measurements were made for a single source location in the near

wake of cube. Drag tank tests (uniform approach flow) reproduced Golden's results, and Snyder established that the Reynolds number must exceed a value of approximately 11,000 in order to obtain a Reynolds-number-independent flow structure for uniform approach flows. Snyder extended this study for shear flows oriented perpendicular to a cube face for a source also released at the downwind base of the cube. He concluded that $Re > 4,000$ would limit perturbations to twice the minimum inherent concentration standard deviation, S , where

$$S = \left[\frac{1}{N} \sum_{i=1}^N (\log K_{i1} - \log K_{i2})^2 \right]^{1/2} \quad [2]$$

and $K_{ij} = O_{ij} UH^2/Q$ is the dimensionless concentration coefficient measured at port i during situation 1, and situation 2 is selected to be a case which definitely exceeds the critical Reynolds number. Snyder chose a minimum S of 0.1 and a minimum discrimination level in K of 0.001. In the Snyder data there may be some influence of the low Reynolds number approach flow on the specified critical Reynolds number since the friction Reynolds number under that experimental condition was low, ie. $Re^* = 0.9 < 2.5$.

Implications for Fluid Modeling Criteria: Based on measurements reviewed above, a fluid modeler would feel justified in performing dispersion experiments in the vicinity of model buildings when the Reynolds number based on building height and upwind wind speed at that height exceeded 4,000. However, these data are limited to flow about cubes, cubes oriented normal to the approach wind, and sources located at ground level in the near downwind wake of the obstacle, $x = H/4$. It was felt these conditions are not necessarily the most severe or complex situations one would encounter during a fluid modeling study; hence, additional measurements were planned for a non-cubic but rectangular prism building shape, orientations other than normal to the approach flow, and source positioned at various roof top locations.

Wind tunnel experiments were performed of dispersion in a boundary-layer meteorological wind tunnel over a range of wind speeds (12 conditions), building orientations (0° - 30°), model scales (1:25 and 1:50), and source release locations (3 sites) by Neff and Meroney (1996). Measurements suggest that, given the complexities of roof source location, orientation, and intermittent reattachment of streamlines on the building surface, flow conditions should be

set such that $Re > 15,000$ to assure Reynolds number independence of dimensionless concentration values on the building surface and in the building wake region (Isyumov, 1999).

3.1 *Modeling of Stack Plumes*

In the early 1900s turbulent jets exhausting into quiescent or cross-flow air streams were studied in wind tunnels. Plume buoyancy effects were recognized but not simulated, and background flow was laminar in character. Authors quickly recognized the importance of exhaust to free stream velocity ratio, but did not generally examine the importance of density ratio, Reynolds number, Froude number, or momentum flux ratios. Sherlock and Stalker (1940) noted plume bifurcation in the cross flow, but attributed the effect to von Karman vortices and deduced incorrectly the horizontal vortices were rotating downward at plume center. Hohenleiten and Wolf (1942) concluded correctly there was an upward motion at the center of the wake. Bryant (1949) and Bryant and Cowdrey (1955) examined the effects of both velocity and temperature of discharge on the shape of smoke plumes.

Among the first to directly address simulation criteria for air pollution aerodynamics were Strom and Halitsky (1954), Halitsky (1962, 1968, 1969), Cermak et al. (1966) and Melbourne (1968). Most experimentalists agreed that to simulate plume or puff trajectory and mixing behavior correctly in the laboratory one must have similarity in approach wind profiles including turbulent behavior, a fully turbulent exhaust jet, and equality of density, momentum, and buoyancy ratios. Unfortunately, simulation of the buoyancy parameter (Froude number) at reasonable tunnel scales implies very low model wind speeds with poor turbulent similarity. The search for an acceptable “partial” simulation has led to many proposals for distorted scaling of density, stack diameter, and exhaust velocities which are not always consistent. Isyumov and Tanaka (1979) compared a number of such schemes, but the suggestions by Snyder (1972, 1981) are most often accepted as the standard simulation criteria.

Jensen and Franck (1963) examined stack shape and velocity in their monograph on wind engineering similarity. They examined circular, square, and rectangular combinations to see the effects of multiple flues and exhaust velocity on stack downwash.

Boundary layer meteorological wind tunnels were first extensively used by Cermak and coworkers to study point, line, area, and volume sources in the 1960s and 1970s (Cermak et al. 1966; Cermak 1974). Yang and Meroney (1972) measured the behavior of non-stationary or instantaneous emissions in a turbulent shear layer with a laser-light scattering probe. These data

have been used to calibrate Lagrangian similarity models and characterize the effects of shear on vertical and lateral transport. Similarly, Hibberd and Sawford (1994) used laser induced fluorescence to track plume and mixing layer phenomena in a salt-water analogue to the thermal convective boundary layer process at the Atmospheric Research Division, CSIRO Aspendale, Australia (See section 3.6 for further discussion about fluid modeling and stratified flow situations).

3.2 *Modeling of Plumes Interacting with Structures*

Many early model dispersion studies were concerned with plume interaction with fossil-fuel power plant buildings (Hohenleiten and Wolf, 1942; Sherlock and Stalker, 1940; McElroy et al., 1944; Strom, 1953). They recognized the importance of elevating the plume above a minimum height to avoid immediate entrainment and downwash and the broadening effects of wake turbulence on the downwind plume, but they failed to adjust for the effects of approach wind profile on near building flow, separation, re-attachment and the ground-level horseshoe vortex.

Strom and Halitsky (1954) recognized the need to simulate background turbulence, but tried to solve the problem in an ad hoc manner with the insertion of random-hole turbulence generator boards and laterally oscillating table fans upwind of their models. Needless to say, this produced enhanced turbulence, but of no quantifiable intensity or scale related to the atmosphere. Indeed, even the often-quoted work by Halitsky (1968) primarily reports measurements for uniform approach flow model studies.

Golden (1961) proposed a minimum building Reynolds number criteria for building emission studies above which near-building concentration distributions would be flow independent. He concluded one should maintain $Re = U_H H > 11,000$ where U_H was approach speed at building height H . Strangely, this conclusion was based on measurements in a uniform approach flow from a release at only one building location and data sampled at only one location on the building surface. Nonetheless, this result has been almost universally quoted for nearly 40 years (Slade 1968; Snyder 1981). More recently work by Castro and Robins (1977), Snyder (1992), and Meroney and Neff (1996) have clarified this matter. It is now known that the criteria are affected by source location, building orientation, and measurement location. Simulations for measurement locations in the middle to far wake region ($x > 1H$ downwind) may only require $Re > 3,000$ if a truly turbulent exhaust plume exists. However, surface concentration distributions on the building surface itself may vary with wind speed until Re values exceed 15,000.

Meroney (1982a) summarized progress during the 1970s resulting from fluid model studies, and he provides several simple formulae and figures to calculate first order plume/wake interaction effects on concentrations. Hosker (1984, 1985, 1990) and Hosker and Pendergrass (1987) summarize more recent measurements related to near plume entrainment, wake structure, and the effects of clusters of buildings.

Validation of any plume modeling methodology must depend on direct comparison with prototype measurements. Unfortunately, such joint studies are very limited. In many cases acceptance of results is based on only a few points or just the observation of smoke tracers in the field. The field measurements made around the Phoenix Memorial Reactor at U. of Michigan when compared to wind tunnel measurements by Martin (1965) were among the first to verify that laboratory measurements could be trusted to give reliable predictions. Hatcher and Meroney (1977) and Bouwmeester et al. (1981) compared laboratory and field concentration measurements for plume dispersion near the Experimental Organic Cooled Reactor, ID, and the Rancho Seco Nuclear Power Station, CA. Tests included cases with variable stratification and nonstationary wind fields. A comparative analysis showed that combining wind-tunnel measurements with a statistically weighted algorithm method is 40 times more accurate than the conventional Pasquill-Gifford formulae. Graham et al. (1978) compared wind tunnel and aircraft measurements of terrain induced turbulence and dispersion from stacks at the Kingston Steam Plant, TN. One participating meteorologist (Dr. Peter Sinclair) told me that the results were so similar *“it was probably not even necessary to perform the field measurements.”*

Fackrell and Robins (1982), Li and Meroney (1983a,b) and Wilson (1995) studied intermittent plume behavior about buildings by measuring the concentration fluctuation statistics on building surface and in the wake using fast response concentration katherometers. This led Meroney (1985) to propose a probability based methodology to calculate re-entrainment concentrations about a building. More recently Shin et al. (1991) have extended these early measurements to concentration fluctuations produced by dense gas clouds downwind of enclosure barriers.

CFD prediction of dispersion about buildings has “exploded” in the last ten years since the institution of the Computational Wind Engineering Conferences in 1992, 1996 and 2000. This use is not confined just to the research environment, but is now common in industry. In order to assess the likely extent of solution variability arising from the wide range of possible users-inputs and decision (e.g. meshing choices, turbulence models, boundary conditions, etc.)

several projects were initiated to examine variability over a wide range of typical structural and topographical situations. Meroney et al. (1998) considered whether an engineer with typical consulting experience could produce reliable dispersion predictions using an “off-the-shelf” commercial code and modest training. They concluded qualitatively correct predictions contained significant quantitative differences from reality. Cowan et al. (1997), Robins (1998), Castro and Graham (1999), Castro et al. (1999), and Robins et al. (2003) reflect the conclusions based on extensive comparisons of fluid modeling and CFD comparisons of such studies during the European Union Project EMU. They concluded significant variability in comparisons could be introduced by human factors (familiarity with the CFD code), mesh construction, source conditions, turbulence models, inlet conditions, and representation of the geometry (ad hoc choice of building and terrain simplifications). They felt their most important point was that the ‘best’ CFD solution was not necessarily the same as that from the experiments because of turbulent modeling inadequacies. Consequently a coarse mesh model sometimes produced better agreement with observations than a fine mesh model. Stathopoulos (2002) also expressed skepticism about CFD simulations of plume interaction with structures. He concluded that “in spite of some interesting and visually impressive results produced with CWE (Computational Wind Engineering), the numerical wind tunnel is still virtual rather than real, and many more parallel studies – numerical and experimental – will be required to increase the level of confidence in the computational results.”

Although the overall ability of CFD modelers to reproduce experimental bluff-body case studies is not impressive, there are several examples of successful validation. Even some of the current critics have produced computational predictions in good agreement with experimental data. Li and Stathopoulos (1998) reported “good agreement” for predictions of longitudinal ground-level downwind of simple prisms studied in a wind tunnel. Meroney et al. (2000) reported good comparisons between numerical and flow modeling of boundary layer flow and wind loads on hemispherical shaped structures. Hangan (1999b) claimed “mild” agreement between the CFD and wind tunnel simulations for the vertical, stack-type releases over a building.

3.3 *Modeling and Natural Ventilation*

Flow visualization through model buildings has frequently been used to evaluate the effect of natural air movement through windows and doors and forced circulation from heating and air

vents. Smith (1951) describes an airflow chamber constructed to study fenestration flow patterns. They compared flows through a 10 m full scale building constructed on a rotating turn table to a 1/15 scale model. They found to their surprise that changes as small as 3mm in model window ledge design could completely change internal flow fields. Subsequently, many case studies showing flows around and within different shape structures were reported by Caudill et al. (1951), Caudill and Reed (1952), White (1954), and Evans (1957). Ventilation studies inside industrial style buildings are recorded by Baturin (1972).

Outdoor air moves through a building either due to intentional ventilation (natural or forced) or unintentionally due to infiltration (and exfiltration). Net air exchange in buildings is typically modeled by empirical models based on statistical evaluation of pressurization tests or by semi-empirical models that sum contributions from individual building components. The local building surface pressures due to wind or thermal effects (stack) are estimated from wind tunnel tests (Dick 1949; Straaten 1967; Aynsley 1985). Unfortunately, such methods can not normally account for the effects of wind gustiness, internal pressure fluctuations, or sheltering.

Ventilation rates can be determined from model tests in wind tunnels either by measuring the external pressure distributions and using this data for a theoretical prediction or by measurement of ventilation rates directly. A strong argument for direct measurements is that theory does not account for effects of wind turbulence and internal air movements. Ohba et al. (2001) presented data from a wind tunnel program to examine cross-flow ventilation through a simple rectangular building including finite size window and door openings. Their intent was to develop a data set suitable to calibrate future CFD programs. Unfortunately, it is hard to specify the actual leakage paths, and it is generally argued that it is not possible to achieve full-scale Reynolds numbers in model cracks at model scale. Birdsall and Meroney (1995) measured rates of wind-forced infiltration and natural convection into a scale model of the Texas Tech University Wind Engineering Research Field Laboratory building (TTU WERFL). Meroney et al. (1995) describe an alternative infiltration model strategy that permits simulation of instantaneous flow rates as $Q/(AU)$ for both infiltration and dominant opening flows. Linden (1999) reviews model work examining the joint effect of natural ventilation and buoyant air flows within rooms. Nishizawa et al. (2004) presents a comparison between the Japanese Building Research Institute wind tunnel and CFD results for a full-scale building. The building had equal sides of 5.56m and a height of 3 m and was divided into 4 rooms with associated doors and window openings. The authors used the commercial code STREAM to calculate velocity,

turbulence and flow direction fields. Comparisons were made between velocity fields, pressures over the building facade, and ventilation rates within the building. They concluded wind fields were similar, calculated pressure coefficients were slightly lower than measured (80-90%), and ventilation rates and differential pressure between openings were quite good, but the authors felt data correlations could improve with an alternative turbulence model.

The unique nature of ventilation applications have led to specialization in CFD software with programs designed to specifically model features of inlet and exhaust ventilators, energy sources like people, computers, and lights, solar radiation, etc. (e.g. FLUENT Airpak, Flomerics Flovent). These applications have also led to extensive measurement programs to validate numerical modules within these programs (e.g. Faber, 1999; Schwarz, 2003). These same programs have also been applied to wind engineering applications including plume dispersion about urban building centers, industrial complexes, vehicle tunnels, etc. (Alamdari, F., 1994).

3.4 *Modeling of Plumes Interacting with Complex Terrain*

In 1929-30 airflow over the Rock of Gibraltar was studied in a National Physical Laboratory wind tunnel to determine safe takeoff and landing patterns from the local airfield. Subsequent measurement of the actual flows around the Rock of Gibraltar with pilot balloons and kites found that the model “*closely forecast what occurred in nature at Gibraltar, in regard to wind directions and the distribution of vortices and vertical currents*” (Field and Warden, 1929; Briggs, 1963). Also in 1929 Abe used cold CO₂ sublimated from dry ice flowing over a 1:50,000 scale model Mt. Fuji, Japan to study mountain wave clouds. Visualization photographs revealed wave like motions near the model mountain peak that correspond to the presence of laminar wave clouds seen over the actual volcano. Then in 1937 Theodore von Karman consulted on wind tunnel studies of flow over a number of mountainous areas in New England at scales ranging from 1:5000 to 1:8000 to identify good wind power sites to erect the 1500 kW wind turbine conceived by Palmer Putnam (1948). Unfortunately, the researchers failed to consider the effects of the atmospheric shear layer; hence, the results failed to agree with field measurements.

Among the first studies to determine plume behavior perturbed by terrain were those of the Point Arguello and San Nicolas Island, CA, naval weapon test sites (Cermak et al. 1966; Meroney and Cermak 1966). Concern was expressed that toxic plumes emitted from rocket engine test stands might drift over populated areas downwind. These studies were performed

under scaled atmospheric boundary layer conditions and included the effects of stable stratification on plume dispersion. Stable stratification enhanced plume channeling by terrain features and diminished vertical mixing. Extensive field programs of plume motion at both sites were completed. Measurements at Point Arguello agreed qualitatively and quantitatively with wind tunnel values, but the field measurement program at San Nicolas Island never recovered any useable data.

Meroney et al. (1978) and Meroney (1979) compared field measurements of a wind field in the complex Rakaia Gorge region on the southern island of New Zealand to an array of wind tunnel models at a 1:5000 scale with different surface textures including stepped terrain, smooth terrain and vegetated terrain. They found that inclusion of surface features including individual tree lines was crucial to satisfactory simulation of the boundary flow separation and reattachment over the terrain. Laboratory and field measurements of wind speed and direction were found to agree within sample correlation coefficients of 0.70 to 0.76 and 0.65 to 0.67, respectively. Rank correlations between relative wind speeds over the field site and model agree within 0.78 to 0.95.

Joint field and wind tunnel tests of dispersion during valley drainage flows were considered by Yingst et al. (1981). Dispersion over the Geysers Geothermal area, Ca. was simulated using 1:1920 scale models where surfaces were cooled with dry ice. Results compared well for both neutral and drainage flow situations. Weil and Cermak (1981) examined dispersion from a paper plant in a river valley under stable stratification. They found comparable values of dimensionless concentration in the field and laboratory.

Meroney (1980a, 1980b, 1990), Cermak (1984) and Snyder (1985) reviewed the success of terrain flow simulation and associated dispersion experiments. Experiments have been performed in both water and wind tunnels with and without thermal stratification. Simulation criteria and tunnel size place a strong constraint on the ranges of permissible scales and dispersion distances examined. Falvey and Dodge (1977) performed a unique experiment for estimating the dispersion of ground-level generated weather modification nuclides over western Colorado by accounting for Coriolis effects in a stratified rotating water tank simulation. Their measurements explained the unanticipated distributions found during prior field experiments, which are associated with Coriolis driven modifications to mountain-valley flows. Studies included simulations of the Leadville-Climax, San Juan, and Sierra Nevada regions in Colorado.

In related studies on predicting wind energy over complex terrain, Meroney (1993), Meroney et al. (1993a, 1993b) and Neff (1993) considered the combined effect of vegetation

height variation and hill shape on the atmospheric boundary layer. They found that vegetation height and extent significantly influenced the location and extent of local separation regions on isolated two-dimensional hills, and that the height and location of upwind hills can also radically alter the wind profiles of downstream hills. Bitsuamlak et al. (2004) recently prepared a review of fluid and computational modeling of flow over complex terrain.

3.5 *Modeling of Plumes Interacting with Vegetation*

The earliest measurements of wind flow about vegetation were performed to evaluate crown form and blow down of young tree plantations, not atmospheric dispersion (Tiren 1927). Later tests were also performed to determine vegetation effects on wind profiles related to wind energy prospecting (Meroney 1993). But during the 1960s the US Army supported an extensive wind tunnel program at Colorado State University of flow and dispersion within and above agricultural canopies (e.g. Plate and Cermak 1963; Plate and Quareshi 1965; Kawatani and Meroney 1970). Models were constructed of both stiff and flexible crops (corn vs wheat) using arrays of pegs and flexible plastic strips. Model forests were represented by artificial plastic trees. The specific model trees were chosen based on drag and wake profile measurements made about small live trees inserted into a wind tunnel (Meroney 1968). Concentration measurements were used to develop analytic and numerical models to predict penetration of gaseous plumes into and within canopies during insect and herbicide spray programs.

Amorin et al. (2004) computed the flow over Lisbon, Portugal, and dispersion from traffic sources with and without the influence of street side vegetation using the FLUENT Code. Their model included an extended region of urban structures and streets and calculated CO dispersion over a full 24-hour day. Comparisons of field measured to model predicted levels of CO produced standard correlations of 0.912 when vegetation was included versus 0.589 when vegetation was excluded from the numerical model. Meroney (2004a) represented both forests and urban street canyons as a simple porous media to calculate the relative movement of fire and smoke plumes set at different locations within the canopies. He found significant differences in the relative growth and rise of plumes for fires located on flat unobstructed planes versus those located within the porous canopy.

3.6 *Modeling of Plumes in Stratified Environments: Stable and CBL Situations*

Most dispersion incidents produce maximum surface concentrations during either stable or unstable stratification. Stable flows lead to plume trapping, plume channeling in complex terrain, plume impingement, and transport of undiluted gas streams far downwind. Unstable flows lead to plume fumigation, adverse descent of elevated plumes to the ground and lift-off of ground level plumes. A number of wind tunnel facilities have been constructed worldwide to focus on the effects of stratification on dispersion (Cermak 1974; Meroney 1998a). Laboratory dispersion tests performed in Australia, England, Germany, Japan and the USA forcefully demonstrate the extent and importance of such phenomena.

Arya (1968) and Ohya et al. (1997) defined the character of stably stratified boundary layers based on wind tunnel measurements of velocity profiles and turbulent spectra. The behavior of continuous gas plumes emitted into a stably stratified boundary layer was studied by Chaudhry and Meroney (1973) who used Arya's boundary layer configuration.

Meroney et al. (1975) simulated the influence of stably stratified flow over a heated shoreline to estimate plume fumigation downwind of a shoreline power station. Later, Avissar et al. (1990) examined conditions required to permit joint numerical and laboratory simulation of sea-breeze type phenomena. Kothari et al. (1985) considered the dispersion of gases released into the wake of a model building immersed in a stably stratified flow field. Stratification induced significant changes in the plume entrainment and the growth of the perturbed wake. Orgill (1971) predicted the dispersion of silver-iodide weather modification nuclides in the Colorado River valley and near Wolf Creek Pass, CO. Grainger and Meroney (1993) examined the dispersion in large open-pit coalmines during night-time inversions situations. Strong stable stratification could lead to dangerous fume trapping in the pit that is hazardous to mine operations.

Although Willis and Deardorff (1974) considered convectively driven dispersion in their stratified water box experiments, the inclusion of cross flows and boundary layer shear has only been examined fairly recently. During the late 1980s and 1990s teams at Colorado State University, USA; U. of Karlsruhe, Germany, Monash University and CSIRO, Australia have examined ground and elevated source dispersion under unstable stratification convective boundary layer (CBL) conditions in special wind tunnel and water channel facilities. Meroney and Melbourne (1992) presented simulation criteria for CBL situations, and they provided performance envelopes which indicated appropriate simulation ranges for different laboratory

facilities. These equipment and measurements are described more fully in the NATO monograph on *Buoyant Convection in Geophysical Flows* (Plate et al. 1998).

3.7 *Modeling of Plumes in Urban Environments*

The NATO monograph on *Wind Climate in Cities* provides a good starting point to consider the interaction of the urban environment and plume dispersion (Cermak et al. 1995). Early studies considered generic arrangements of building clusters and streets to determine the influence of street and building alignment on traffic exhaust dispersion (Hoydysh et al. 1974; Wedding et al. 1977; Cermak, 1978). Some experiments included the option of multiple moving vehicle sources (Kitabayashi et al. 1976; Thompson and Eskridge 1987). Others chose to simulate street level sources with line sources (Meroney et al. 1995, 1996; Schatzmann et al., 1997

Most such model studies are performed to help design numerical air pollution models suitable for calculating extreme air pollution episodes due to combined fixed sources and vehicular sources. Klein et al (1994) designed a study to monitor dispersion about a U-shaped building specifically to critique modules in air pollution models used to adjust for air pollution aerodynamics. Leidl et al. (1997) compares the results of various model calculations against the U-shaped building laboratory data.). Rodi (1995) reviews the CFD experience with simulation of flow around single and groups of buildings using statistical turbulent models (RANS type).

Simulation of urban dispersion using CFD has become increasingly ambitious. Simulations began with flow about single cubes immersed in a boundary layer, later flow over groups of buildings (4-8) were modeled, and today calculations consider flow and dispersion over entire urban districts including vegetation, lakes, solar radiation and vehicle traffic. Urban street canyon studies have ranged from 2-dimensional simulations (Leidl and Meroney, 1996; Xia and Leung, 2001) to full 3-dimensional predictions including multistory buildings, and moving traffic sources. Murakami et al. (2000) proposed a protocol to examine how mesoscale weather predictions can be extrapolated down through a series of nested grids to urban, district, street and interior ventilation conditions.

Previously in Section 3.6 we considered how Amorin et al. (2004) successfully predicted street pollution in Lisbon city including vegetation effects. Nakayama and Tamura (2004) have recently used a LES turbulent model approach to predict fluctuating windflow and dispersion across two different 1 km x 1 km districts in Tokyo. One was predominantly suburban and the other included regions of high-rise buildings. Although they had no field data comparisons, they

presented the results of a validation exercise using the same numerical procedure comparing predictions to flow over a normal plate (or fence) in a wind tunnel boundary layer.

3.8 *Modeling of Dense Gas Plumes*

Bodurtha (1961) examined visualizations of the behavior of dense gas plumes in a wind tunnel shear layer to evaluate the plume trajectory and dispersion of gas-relief valves. Hoot and Meroney (1974) measured concentration fields produced by dense plumes emitted into quiescent air and cross-flowing boundary layers. They fit their data to equations derived from integral plume analysis, and proposed relations to calculate plume trajectory, ground touchdown locations, and subsequent surface concentrations (See Bodurtha, 1980).

Concern about safety issues associated with the storage and transport of liquefied natural gas (LNG) led to an extensive field and laboratory program on dense gas dispersion during the 1970s and 80s. Large field experiments were performed at China Lake Naval Weapons Test Center, CA and the US Dept. of Energy Field Site, NV, as well as at Porton Downs and Thorney Island, UK, and in The Netherlands. Many of these tests were selected for co-simulation in world wind engineering laboratories (CSU, USA; Warren Springs, UK; EPA Fluid Modeling Facility, USA; U. of Karlsruhe and U. of Hamburg, Germany; TNO, The Netherlands). A summary of such experiments are described by Meroney (1982b, 1987) and Shin and Meroney (1989). A review of modeling criteria necessary to simulate dense gas plumes including buildings and terrain may be found in Meroney (1986a,b, 1988).

The interaction of dense gas clouds and water spray curtains was examined by Meroney et al. (1984). The study successfully simulated releases of dense CO₂ clouds performed by the Health and Safety Executive, UK. Later Shin et al. (1991) replicated in a wind tunnel the time-dependent dispersion observed during the Falcon Test Series including the joint effects of barriers and water-spray curtains.

Laboratory studies continue to be a primary source of data for safety analysis in the petro-chemical industry due to the cost and complicated nature of successful field experiments. Recent references incorporating the results of fluid modeling related to air-pollution aerodynamics and industrial safety include Fannelöp (1994) and Hanna and Drivas (1996). During the middle to late 1990s the Petroleum Environmental Research Forum (PERF) made up of nine major oil companies worked with the U.S. Department of Energy (DOE) and the U.S. Environmental Protection Agency (EPA) to support a dense gas dispersion modeling project

(Hanna and Steinberg, 2001). This project supported a coordinated set of wind tunnel experiments at four wind tunnel facilities and a set of dense gas field experiments (Kit Fox) at the Frenchman Flat area of the U.S. Nevada test site. The results from the experiments were used to validate stratified mixing expressions used in the DEGADIS, HEGADAS and SLAB predictive models. These models are all depth integrated models which solve differential equations for lateral plume spread and characteristic vertical growth. Principle results are provided in papers by Meroney (1989), Robins et al. (2001a, 2001b), Snyder (2001), Briggs et al. (2001) and Havens et al. (2001).

3.9 *Modeling of Fire and Smoke Pollution*

Predicting smoke and flame behavior can be based on full-scale field experience, analytic integral approximations that capture the gross flow behavior, fine-scale numerical modeling and/or physical modeling at reduced scale...these methods are typically called full-scale, zone, field (numerical), and physical modeling, respectively.

Williams (1969) identified twenty-nine dimensionless groups required to simulate large fires based on normalization of the governing equations of motion, energy and concentration. A subset of eleven dimensionless groups was considered important, and seven were designated as critical for even partial simulation:

- Geometrical similarity,
- Convection (Reynolds number),
- Radiation groups (2) (Ratio of L to radiation absorption length and blackbody radiation flux to enthalpy convection),
- Gas-phase heat release (enthalpy of formation to ambient enthalpy),
- Fuel gasification energy (total heat required to gasify a unit mass of fuel to ambient enthalpy), and
- Fuel loading or burning rate group (Time average mass burn rate to convective mass flux);

Of lesser importance were dimensionless ambient velocity, vorticity, and atmospheric lapse rates. These dimensional considerations lead to several possible strategies for simulating mass fires.

Standard scaling: Keep some groups constant. Usually Froude number and Mass burning rate are chosen which leads to distortions in radiation, convection, turbulence and fuel bed geometry. Basically one is just looking at a buoyant plume.

Pressure adjustment: Varying pressure might preserve scaling of all but radiation parameters. Unfortunately to scale a 1 mile fire to 50 feet would require use of a facility able to withstand a pressure of 1000 atm.

Pressure and body force adjustment: Varying pressure and G (centrifuge) simultaneously allows consideration of all core variables except blackbody radiation.
Adjustment of composition and temperature of ambient atmosphere: Varying pressure and temperature could permit scaling of all core variables except absorptive radiation.
Adjust pressure, temperature and body force: All core variables satisfied, but maximum LSR variation probably limited to about 10.

The conclusion must be that satisfactory physical model scaling of all aspects of mass fires is not likely.

Froude modeling (Fr) using either air or saltwater is probably the most common kind of physical modeling for hot smoke transport. Smoke movement away from the vicinity of a flame can be reproduced, but chemical kinetics, flame dynamics, and heat transfer scaling is not preserved. Unfortunately, due to scaling constraints it is difficult to simultaneously simulate buoyant plume movement and wind induced pressure distributions about the external urban building envelope. Nonetheless, physical modeling has been successfully used to study flow through forest and urban canopies in the absence of fires, and with fires for flow and fire movement through ground litter, idealized ignition concepts, fire whirl dynamics and compartment fires. Quintierre (1989) provides a variety of examples of how physical modeling has been used to model various aspects of fires including: simple fire plumes, ceiling jets, burning (pyrolysis) rate, flame spread, and enclosure fires. Heskestad (1975) includes cases of sprinklered fires. (Also see Gani and Williams, 1992; Quintierre, 1989; Klote and Milke, 2002a; Heskestad et. al., 1983)

There have been extensive studies in fire wind tunnels of fire propagation through porous fire beds made of a variety of different depths of natural and artificial materials. Unfortunately, little of this work is directly applicable to the simulation within urban fires or forests including crown fires. One minor exception is the limited work of Lee and Otto (1975).

In urban areas, buildings of various shapes and heights are grouped together to form city blocks separated from each other by the open streets. Consequently, fire propagation is strongly affected by the unique relationship of the buildings. Lee and Otto (1975) chose to simulate how fires develop about just two rectangular buildings simulated by identical woodpiles of length L , width $L/2$ and height $L/3$ with the long sides parallel to each other. These fuel piles were separated by a distance $L/2$ with an overlap of equal magnitude. The wood cribs were set afire at the same time, and velocity, temperature, and heat flux measurements were made, while ordinary and infrared photography were used to monitor the flames. The fire developed in five stages related to heat flux levels as noted below:

- During Stage 1 both piles burned independently, ambient indrafts were controlled by each pile separately with no evidence of gross vortex activity.
- During Stage 2 the heat flux became strong enough to produce weak interaction between the induced airflow about the two fuel piles. Discretely separate multiple fire whirls extended from each corner. Individual fire whirls strengthened and heat flux increased.
- During Stage 3 the individual whirls of each pile coalesced almost instantaneously into one single flame leaning towards the open street with a single strong vortex column.
- During Stage 4 the vortex became so strong that flames were actually drawn out from the openings on the opposing sides of the piles facing the streets towards the vortex column. Heating no longer occurred primarily in the vertical, but lateral and horizontal heating caused fire to move along the model building. Secondary vortices appeared.
- During Stage 5 the fuel was exhausted, the piles started to collapse, the main vortex column dissipated, and vortex shedding into a wake region predominated. The vortices shed so frequently and violently that this may indicate a primary period of fire spread to other structures.

The interaction of the fire between the two structures that resulted during fire whirl formation and subsequent sucking of flames out of openings (windows and doors) is similar to that assumed by the Himmoto and Tanaka (2002) fire propagation model.

As noted earlier a number of wind tunnel studies have examined flow within arrays of building like blocks placed in arrays to simulate generic and actual urban districts. Cermak (1995) concluded that the general nature of above city flow including distributed roughness and the effects of the heat island can be simulated when Richardson number similarity exists and for sufficiently large model Reynolds numbers. Plate (1995) and Theuer (1995) demonstrated that similarity of flow exists for a wide range of roughness arrangements including actual city geometries. Quintela and Viegas (1995) and Meroney (1978) concluded that even thermal effects to buildings can be simulated given equality of the parameter $Re/(Gr)^{1/2}$. Finally, dispersion of neutrally buoyant scalar plumes from point or line sources, which might represent the dispersion of cool smoke, was studied by Theurer (1992, 1995), Meroney et al. (1996), and Chang and Meroney (2003). No additional examples of intense heat sources or actual fires released within physically scaled model forest or urban environments are known to this author.

On the other hand, attempts to model compartment and exterior building fires are numerous, such that Friedman (1992) produced a survey of some 31 zone models and 10 field models for compartment fires. He also summarized some 12 models for fire endurance, 6 models for building evacuation, 5 models for actuation of thermal detectors, 3 models for fire-sprinkler interaction and 7 miscellaneous models for mines, wall fires, and window plume fires.

The foundations for the U.S. NIST Fire Dynamic Simulator (FDS) field model are described by Baum et al. (1997). This versatile model allows simulation of fire combustion, smoke dispersal, radiation, heat transfer and even considers the effects of water sprays (See description and download at <http://www.fire.nist.gov/fds/>). It has been extensively validated with full-scale and fluid modeling experiments. Klote (1999) simulated the effects of HVAC induced flows on smoke response using the commercial CFX code. Hadjisophocieous and Lougheed (1999) used the code TASCflow to compare computations of flow movement in atrium smoke exhaust systems to experimental results in a small and large scale fluid modeling facility. Sanquer (2002) examined flow through smoke ventilators using full size, model and numerical evaluations. In a “hybrid” approach she used numerical and fluid modeling to provide a critical analysis of the recommended full-scale test procedures.

Meroney (2002) and Meroney et al. (2002a, 2002b) modeled the movement of fire and smoke within large building atria using the FLUENT code. They validated their computational procedure against published data for flow, temperatures and smoke levels in experimental fire chambers. During numerical calculations prepared to help architects design a proposed building atria, fire whirls were observed to develop during the unsteady simulation of a fire. Subsequently, Meroney (2003) was able to duplicate laboratory measurements of the time dependent growth of additional fire whirls using the CFD code. Finally, Meroney (2004a) reviews the subject of fires in urban and forest settings and calculates the initial growth of large-scale fires developing in urban/forest canopies using a simple porous media approximation to the presence of the distributed buildings and trees.

3.10 *Modeling of Droplets, Drift and Particles*

Rain or spray simulation (droplet diameters = 100 to 6000 microns). Wind-driven rain (WDR) or driving rain considers droplets that are given a horizontal velocity component by the wind. WDR is the most important moisture source affecting the durability of building facades. The displacement of raindrop trajectories by buildings, trees and terrain is also very significant in hydrology, the design of rainfall networks, and soil erosion. Blocken and Carmeliet (2004) review the current state-of-the-art in WDR research for experimental methods, semi-empirical methods and numerical methods. Rain penetration has sometimes been predicted based on the surface pressures measured across rain screens during fluid modeling experiments; hence, in such cases no rain simulant is required. But problems involved in model scale simulation of

actual rain are significant. These problems include 1) variations in intensity and droplet size distributions during a storm, 2) interaction of the water droplets with building-induced flow patterns, 3) generation of appropriate size distributions artificially with nozzles, 4) evaporation of droplets during their fall, 5) water droplet distributions on the building facade, and 6) migration of the rain as films or shattered droplets (splash) down the building facade.

Surry et al. (1994) attempted to address problems 2 through 6 in a directed research program in the wind tunnel facilities at the Boundary Layer Wind Tunnel Laboratory (BLWTL), University of Western Ontario, Canada. The primary purpose of their rain shower experiments were to determine the effect of rain impingement on pressure variations across compartmentalized rain screens which might lead to degradation of performance and leakage inside the building facade. They concluded a model simulation could be accomplished if one simulates the natural wind characteristics, the ratio of droplet terminal speed to wind speed (fall angle), and Froude number. It is generally agreed that even intense rain does not significantly modify the wind field and individual droplets are well separated. Surry et al. (1994) found that they could approximate a desired rain fall distribution using discrete spray nozzles with overlapping sprays at a scale of 1:64. Actual rain intensity was measured using sensitive paper that showed stains on rain impact, but unfortunately the counting and sizing of individual stains is very labor intensive and tedious, is limited to very short test periods (~10 seconds), and shows large test to test variability. Blocken and Carmeliet (2004) conclude that fluid modeling may be no less demanding than field measurements with no guarantee of increased accuracy.

Sprays are also used to distribute herbicides, fertilizers, and insecticides, to wash automobiles, to mitigate fog or ground level inversions over fruit crops or airport runways, or to coat objects with paint. Heskestad et al.(1983) describe fluid modeling experiments performed to quantify how water sprays can dilute flammable gases during a liquid natural gas (LNG) spill. Meroney et al. (1984) and Meroney and Neff (1985) developed a depth integrated CFD model to predict the effectiveness of such water sprays in mitigating hazards associated with LNG spills and calibrated their model against field data U.K. Health and Safety Executive tests on the water spray dilution of heavy CO₂ clouds.

Choi (1993, 2000) and Blocken and Carmeliet (2000, 2002) simulated wind-driven rain around a building by first computing the flow field around the building and then using Lagrangian predictions of droplet trajectories influenced by drag induced by relative flow and droplet motions. Hangan (1999a) compared FLUENT CFD predictions of rainfall to a wind-

driven rain impact on buildings studied in the BLWTL facility at the University of Western Ontario. He reported fairly good agreement between CFD and experiments in terms of local intensity factors (LIF - the ratio between the rainfall intensity on a certain building zone to the undisturbed rainfall intensity). Blocken and Carmeliet (2002) provided full-scale experimental verification of the method on the low-rise VLIET test building in Heverlee, Leuven. The building has both sloped and flat roof segments, is situated in a suburban area, and was instrumented with nine driving rain gauges positioned on the building envelope. The numerical program reproduced both the temporal variation and magnitude of rain catchment over the building and highlighted the effects of roof-overhang sheltering, blocking provided by sloped roofs, and the selective disturbance of droplet trajectory based on droplet size.

Droplet or drift simulation (droplet diameters = 1 to 1000 microns). Drift particles (or droplets) included with emissions from stacks or cooling towers are brought to the surface through the combined processes of turbulent diffusion and gravitational settling. Once near the surface, they may be removed from the atmosphere and deposited on the surface. Although the background flow fields and gaseous plume motions may be accurately predicted by physical modeling in environmental wind tunnels at moderate velocities, the correct scaling of droplet and particle drift requires that the simulations be run at extremely low facility velocities, which then distorts the model flow fields (Kennedy and Fordyce, 1974; Jain and Kennedy, 1978; Petersen, 2004). The trajectory and diffusion of the water vapor plumes (without associated droplets) from cooling towers have been simulated in wind and water tunnels (Jain and Kennedy, 1978; Andreopoulos, 1989).

CFD was used to predict water vapor transport from stacks and cooling towers to define plume visibility (England et al., 1973; Bender et al., 1996; Takata, et al., 1996), but most particle deposition predictions are based on modifications to conventional Gaussian plume models (ISC-3) or ballistic trajectory calculations (SACTI). Meroney (2004b) used the FLUENT CFD code to calculate velocity and turbulence fields downwind of cooling towers and the FLUENT discrete particle model option to calculate Lagrangian trajectories of individual droplets which then accumulate on downwind building and ground surfaces. Meroney validated the ground-level accretion levels against field measurements performed at the Chalk Point Power Station in Maryland in 1977.

Snow simulation (particle size = 0.1 to 10 mm). Wind tunnel experiments using fine particles such as sawdust, mica, sand, borax, glass-beads, activated-clay, and even ice-particles or snow have yielded useful information on the shapes and dimensions of drifts near buildings, roads, and mountain ridges. Some experiments have attempted to satisfy similitude requirements, at least partially. In other experiments, modeling laws have been ignored. The exact similitude requirements for scale modeling of drifting snow problems are not met at small scales because of the large number of modeling parameters that cannot be satisfied simultaneously (Strom et al., 1962; Odar, 1965; Mellor, 1970; Kind, 1981; Iverson, 1980a, 1980b, 1981; Sakamoto et al., 2001).

Many researchers emphasize the importance of $Fr = U / (g (sg-1) L)^{1/2}$, the modified Froude number, where U is a characteristic wind velocity and sg is the specific gravity of the snow relative to air. But Iverson (1980a) argues that for similarity in final drift shape and growth rate a mass-transport rate parameter and an aerodynamic roughness parameter govern drifting behavior:

$$D U^2 / (2 D_p g H) (1 - (U_o / U)), \text{ transport rate parameter,}$$

$$A_1^2 (D_p / H) (U_* / U_{*t})^2, \text{ equivalent roughness,}$$

where A_1 is a dimensionless threshold friction speed (Froude number with friction speed as characteristic velocity), U_* is the surface friction speed, U_{*t} is the threshold friction speed, U_o is the threshold wind speed, D is the air density, and D_p is the particle density.

One major limitation of most snow simulants (e.g. glass beads, sand, borax, walnut shells, etc.) is their failure to cornice during deposition; hence, some researchers have used fine activated-clay particles that have the consistency of talcum powder. The clay particles are very effective at qualitatively modeling snow drift topography and permits cornices, but it is difficult to handle, easily absorbs water and clumps together, and often becomes a health hazard (See Cold Regions Research and Engineering Laboratory web site at <http://www.crrel.usace.army.mil/ierd/snowdrif.htm>). One solution proposed to the similarity dilemma is to use actual snow and ice particles, since then particle Froude and Reynolds number parameters are identical at full and model scale. Sakamoto et al. (2001) developed a novel technique that draws a snow layer placed on a moving sheet into a rotating brush that lofts the snow into the oncoming fan-driven wind. Such a scheme produces fractured ice crystals not snow flakes, and may not account for the full-scale effects of snow aging, coagulation, and temperature and humidity changes on snow characteristics with time.

Typical snow modeling studies include those dedicated to the design of snow control fences (Meroney and Meroney, 1988; Meroney and Tan, 1993; Sakamoto et al., 2001) or drift about buildings (Isyumov and Mititiuk, 1997; Delpech et al., 1998; Thiis, 2000; Thiis et al., 2004; Shuij et al., 2004). Thordarson (2002) describes wind tunnel and numerical simulations of snow drifting around an avalanche dam. The model dam simulated was at reduced scale (1:100), but the drifting particles were produced by snow guns at full-scale size, shape and density; hence, the model velocity was presumed to scale as the square-root of the geometric scale. Numerical calculations performed by the code Flow3D at both full and model scales did not actually simulate snow movement just the wind field. Thordarson concluded based on the comparisons that the wind tunnel model probably replicated full scale drifting upwind but not downwind of the dam.

Snow researchers also use CFD as a snow drift prediction tool (Uematsu et al., 1991; Bang et al., 1994; Liston and Strum, 1998; Thiis, 2000, 2004; Beyers et al., 2004). Various models have been proposed to characterize the moving snow and develop drift shapes. Once a flow field was defined by a CFD code, Uematsu et al. (1991) predicted the snow drifting rate by conservation of saltation and suspension. Their method did not calculate actual drift development; hence, it did not consider the changed flow field once a drift became a new obstruction. Bang et al. (1994) used a drift flux model found in the commercial code Flow-3D in which the two phases of snow and air intermingle and the relative motions are determined by pressure gradient driven drag forces. This permits snow to accumulate in regions where atmospheric shear force on the ground surface is lower than the threshold friction velocity for snow movement. Waechter et al. (1997) used a three-dimensional CFD code (TASCflow) to predict the flow field about an actual reference building that exists at the South Pole, then they used available meteorological wind data and an ad hoc finite area element (FAE) computer model (developed by the firm RWDI, Canada based on snow field measurements) which computes snow deposition or scour of snow in a grid of elemental areas. Liston and Sturm (1998) developed the physically based, numerical snow-transport model (SNOWTRAN-3D) to predict snow accumulation over large mesoscale mountain regions. The mass balance equations include effects of deposition and erosion, surface shear stress, saltation, suspension, sublimation, and wind field. The wind field may be generated by several methods including a) applying a physically based full atmospheric model (e.g. CSU RAMS), b) a boundary-layer circulation model, c) an atmospheric model based only on mass continuity (sometimes called a shallow

layer model), d) interpolation of direct observations or e) interpolation of observations in conjunction with wind-topography relationships. The SNOWTRAN-3D model has been validated against a number of winter storm and season snow drift field measurements.

Another possibility is the use of a CFD solver such as FLUENT to determine a wind field and turbulence, and, then, to predict trajectories of falling particles within the wind field by using a Lagrangian discrete particle motion solver to determine particle trajectories and eventual impact and deposition at ground surfaces (Meroney, 2004b).

4.0 HYBRID FLUID AND CFD MODELING OF AIR POLLUTION AERODYNAMICS

Hangan (2004) suggested one call the hybrid approach, the C-FD-E concept. The C-FD-E concept considers the interplay between computational fluid dynamics (CFD) and experimental fluid dynamics (EFD). Hangan argues that the two tools have to play complementary rather than opposed roles in the further development of fluid dynamics. EFD data bases of wind engineering studies of building aerodynamics and dispersion are beginning to accumulate on web sites like the CEDVAL site maintained by the Meteorology Institute, University of Hamburg (See <http://www.mi.uni-hamburg.de/cedval/>) or at the QNET-CFD web site (See <http://www.qnet-cfd.net>) or the NEXUS portal to the European Union ERCOFTAC data base for flow, turbulence, and combustion (See <http://ercoftac.mech.surrey.ac.uk/>). Hangan reports that a new C-FD-E database is under development at the BLWTL at Western Ontario which will emphasize CFD simulations of atmospheric pollution dispersion studies and multiphase/particle flows (See <http://blow.blwtl.uwo.ca/cfd/cfdweb.htm>).

4.1 *Hybrid Case Study: CFD/Fluid Modeling of Stack Diffusion over Rectangular Building*

Predictions of concentrations on a simple rectangular building due to exhaust from a short stack on the buildings roof were obtained by Banks et al. (2003) using flow simulations performed by FLUENT, a Computational Fluid Dynamics (CFD) computer code. These CFD predictions were compared to a database of wind tunnel data for various wind speeds and exhaust parameters. Separate CFD simulations were simultaneously performed at Cermak Peterka Petersen (CPP) and at Colorado State University (CSU) so that the influence of operator decisions could be investigated.

A single 30 cm tall, 60 cm wide, and 30 cm long rectangular model building was placed in an environmental boundary layer wind tunnel section (blockage ~ 2%). The upstream fetch, roughly 15 m long, was covered in surface roughness to produce a coefficient, z_0 , equal to 6 mm (or a suburban roughness of 0.28 m at a scale ratio of 1:50). Tracer gases were released from stacks with inside diameters varying between 7 to 11 mm, flow velocities from the stacks varied from 0.4 to 5.4 m/sec, stack heights ranged between 30 to 90 mm, and wind speed was set to 2 m/sec.

During the blind CFD calculations performed separately by CFD experienced staff at CPP and CSU, the standard k-T turbulence model was used as implemented in FLUENT, but otherwise all decisions concerning creation of the computational domain, domain symmetry, distribution and size of grid elements, entrance velocity and turbulence profiles, and number of grid elements over the test building were specified independently. The CPP calculations were performed over a single domain with solid sidewalls and ceiling and 3400 cells over the test building. The CSU calculations were performed over a single half-domain with a symmetric center plane and 4600 cells over the half building. Both simulations made use of 500,000 to 600,000 cells in total. CSU also chose to use a 15 m long virtual wind tunnel including trips and roughness elements matching the experimental configuration to generate the entrance velocity and turbulence profiles entering the computational domain containing the model building. The CSU method produced velocity and turbulence profiles in equilibrium with the test section roughness, but the turbulence intensity fell off a bit too rapidly with distance above the floor.

Longitudinal concentration profiles along the building surface centerline were compared to experimental measurements and to simple Gaussian plume model, US EPA SCREEN3, analytic predictions. Over the range of conditions studied ($h_{\text{stack}}/H_{\text{building}} = 0.1$ to 0.3 , $V_{\text{stack}}/U_{\text{reference}} = 0.2$ to 2.7 , and $d_{\text{stack}}/h_{\text{stack}} = 0.08$ to 0.37) the CFD calculations tended to overpredict (by factors of 5 to 10) the peak concentration downstream of the stack on the roof and near the top of the rear wall for any case where there was a substantial concentration on the roof. Downstream ground level values tended to look more realistic. The CFD simulation also failed to predict the presence of any stack gas on the upstream side of the roof. The CPP calculation matched the data slightly more closely than the CSU solution, in spite of the use of a coarser grid and less carefully constructed inlet boundary conditions.

This exercise stresses the need for caution when using CFD as a design tool. Even simple configurations need to be validated against experimental data for a similar situation. The

results are consistent with earlier comparisons using RANS turbulence models performed by Meroney et al. (1998) and ERCOFTAC researchers (2000).

4.2 *Hybrid Case Studies: CFD/Fluid Modeling of Urban/Forest Fire Behavior*

Computational fluid dynamics (CFD) provides a design technique to examine the relative merits of various fire suppression strategies. Such programs can inherently consider irregular building and terrain geometry, heat transfer due to variable properties and radiation, time varying fire strength, fire chemistry, effect of fire suppression operation, and variations in weather phenomena. While CFD represents a significant improvement in the predictive capability of smoke control modeling, uncertainties in the predictions remain. The smoke layer boundaries suggested by CFD simulations, just like those of the zone models, are best estimates, and as such have no conservativeness or “safety factor” built in. It is prudent to examine solutions to ensure that they are robust, that is that the flow patterns predicted are insensitive to small changes in boundary conditions such as external wind environment, fire strength, and even fire location. (Klote and Milke, 2002b)

Fortunately, numerical modeling despite its many limitations associated with grid resolution, choice of turbulence model, or assignment of boundary conditions is not intrinsically limited by similitude or scale constraints. Thus, in principle, it should be possible to numerically simulate all aspects of fires within canopies for which realistic models exist for combustion, radiation, fluid properties, ignition sources, pyrolysis, etc. In addition it should be possible to examine all interactions of fire properties individually, sequentially and combined to evaluate nonlinear effects. Thus, computational fluid dynamics may well provide a greater understanding of the behavior of small, medium, and mass fires in the future.

Realistically, however, many of our computational submodules for combustion, radiation, pyrolysis, etc. are still primitive, and even inclusion of all models within a computation becomes cumbersome to calculate, and excessive in use of computational resources and time. Continued verification and validation is required at almost every level of CFD prediction. These caveats notwithstanding, there does exist exciting progress in the use and interpretation of numerical predictions of fire behavior.

Baum and McGrattan (1999) considered a fire growing from the exposed top of an oil storage tank in a 3 x 3 matrix of large cylindrical tanks. Each tank was 84 m diameter and 27 m high. The geometry was chosen to represent a portion of the oil storage facility of the Japan

National Oil Corporation at Tomakomai. A approach velocity profile with a power law distribution of 0.15 and a wind speed at tank height of 6 m/s was stipulated. They used the LES program FDS to calculate time dependent combustion, plume rise, and radiation exposure of the nearby tanks. The model included the effects of radiation from smoke particle back to tank surfaces.

Morvan and Dupuy (2001) predicted fire propagation in Mediterranean shrub land by representing the vegetation as a collection of solid fuel particles distributed with appropriate size, moisture content, density, etc.. Separate layers were created to represent ground cover, crown canopy regions, thinning, and fire breaks. The model captures the degradation processes (drying, pyrolysis, char combustion) and ignition. Calculations were performed over a domain 5 m tall by 20 m long. The authors considered different cell sizes (5, 10 and 20 cm) and compared rate of spread, mass fluxes, contributions of radiation and convection. The model predicted the temperature and velocity field for fires with canopy top wind speeds of 1 and 5 m/s. Their model is intended for incorporation in the EU FIRESTAR system forest fire prediction tool.

Researchers are beginning to add complex terrain into their predictions of fire-spread behavior. Viegas (1998) calculated fire spread rates over a simplified canyon geometry consisting of a horizontal plane and two inclined planes that intersect each other along a line that exists in the vertical plane. Canyon centerline slopes varied from 16.1° to 30° . A constant heat flux over a small area represented a fire at the base of the canyon. A fire propagation algorithm was incorporated in the flow field to estimate the movement away from the ignition point at the base of the canyon. It was found that fire driven convection processes modified the shape of the thermal plume depending on the ambient wind speed and fire intensity.

Coen and Clark (2001) coupled a fire model into a three-dimensional non-hydrostatic terrain-following numerical mesoscale model developed at the US National Center for Atmospheric Research, Boulder, CO. The model includes rain and cloud physics. Calculations predict the growth and spread of a fire line moving across a two dimensional small Gaussian hill (height 200 m, half-width 300 m) at a wind speed of 3m/s, and a stable atmospheric lapse rate (10° C/km). The head of the fire propagated quickly uphill in the direction of the environmental wind. Once the fire reaches the top of the hill, the updrafts tend to inhibit the forward movement of the fire front, and the fire spreads faster laterally in the lee of the hill.

4.3 Hybrid Case Study: Cooling Tower Drift

Results from the Chalk Point Dye Tracer Experiment are described in papers and reports by Hanna (1978) and Policastro et al. (1978, 1981a, b). These experiments are considered to have produced the best single source cooling tower deposition data available. Two natural draft hyperbolic cooling towers are located on the site on a peninsula that extends into the local bay and wet lands. The two towers and the turbine building are located along a east-west line each separated from each other by about 500 ft. The hyperbolic cooling towers are 400 ft (124 m) tall by 374 ft (114 m) diameter base by 90 ft (27.4 m) diameter exit.

Field Experiment 16 June 1977: During the evening of 16 June 1977 Rhodamine WT (fluorescent) dye was added to the cooling tower basin water, and makeup and blowdown valves were closed. Consequently the only loss of dye was through drift loss, and the concentration of dye in the water remained constant for the duration of the experiment. Measurements were made at night during 93% humidity, so there was negligible droplet evaporation. Predominant winds were from the south at 170° ; hence, building and tower wakes did not intersect in the near field. The wind speed profile was in two layers: above 100 m, the wind speed was nearly constant with height, averaging about 8 m/s; below 100 m, the wind speed was nearly linear with height with a mean value of about 5 m/s. Instruments to measure drift deposition were placed at 5° intervals on 35° arcs at distances of 0.5 and 1.0 km north of the cooling towers.

CFD Simulation of 16 June 1977 Conditions: A CFD experiment was prepared to replicate the Chalk Point results using FLUENT (Meroney, 2004b, 2004c). The intention was to validate the DPM accretion option against field data before using the approach in a more complicated building environment.

Calculations for the Chalk Point Cooling Tower simulation were performed on a domain 2000 m long, 1000 m wide and 500 m height using 165,000 tetrahedral cells. The simulated hyperbolic cooling tower height was 124 m, radius of the tower exit was 27.4 m, and plume vertical exhaust speed was set to 4.5 m/sec. Plume buoyancy was included by setting the plume virtual ambient temperature to 295.3° K, and the virtual exhaust temperature was set to 315.3° K. Virtual temperatures were used to account for water vapor content and ambient humidity (Hanna, 1978). To represent the cooling tower drift behavior discrete particle model (DPM) conditions were specified to be a) Particle material was liquid water, b) Particles were specified to be inert

with no evaporation effect, and c) the total flux of sodium from the tower was estimated to be 1.86 g/sec. Rosin-Rammler particle distributions were predicted based on a particle mean diameter of 0.09 mm and a shape factor of 0.65.

Results of Chalk Point Validation Exercise: Heights of the centerline of the cooling tower plume were determined based on the height of the maximum in the water vapor and temperature profiles downwind of the cooling tower. The calculated points agreed very well with the predictions of the Briggs plume rise formulae calculated by Hanna (1978) as well as with the trend of the visual observations for plume height recorded during the experiment.

Predictions of water vapor isocontours in terms of log K factors ($\log C^*U_{ref}/Q_{source}$) were compared to ISCST3 calculations. Ground level values are very low at the edge of the plume and quite sensitive to the assumed cross wind velocities. (Wind velocities were measured to range between 6.5 to 8 m/sec over the region between 100 to 200 m above the ground through which the cloud rises over the first 1000 ft downwind.). Ground level and plume height concentrations were found to agree with ISCST3 calculations.

Accretion magnitudes were compared as observed, calculated by CFD, and analytic values predicted by ISCST-3 and Hanna (1978). The FLUENT computations did reproduce the field measurements within acceptable limits (within factor of 3). Indeed average accretion agreed within factors of 0.75 and 0.5 at 0.5 and 1.0 km, respectively

4.4 *Hybrid Case Study: CFD/Fluid Modeling of Fire Whirls*

Byram and Martin (1962) used external vertical cylinders with tangential slots oriented to produce rotating flow about a fire source. They examined two sets of equipment of diameters and heights, 33 and 183 cm, or 66 and 335 cm. Burning alcohol pools within their apparatus, they reported visible fire whirls up to 300 cm tall with inner fire tube columns 2 cm in diameter. They observed horizontal velocities at the surface of the inner column of about 9 m/sec (~6000 rpm) and vertical velocities to 18 m/sec.

Emmons and Ying (1966) used the rotating-screen apparatus described above to systematically evaluate the effects of angular rotation (Rossby number) and plume buoyancy (Froude number) on fire whirl dynamics. They reported that turbulent mixing coefficient decreases with increasing angular momentum, and increases with elevation above the ground. Later Chigier et al. (1970) reproduced their apparatus but used a turbulent jet diffusion flame.

Since these early experiments several investigators have re-created similar laboratory apparatus while evaluating the character of fire whirls (Martin et al., 1967; Muraszew et al., 1979).

More recently Satoh and Yang (2000 a, b) produced laboratory scale fire whirls by adjusting symmetrical vertical gaps separating the square vertical bounding walls surrounding a central fire pan . They examined the effect of gap size, wall height, fuel size, and heat load on the fire whirl. They determined that there is a critical gap size, which is not so large or small that it inhibits the entrainment of air needed to sustain the fire. Stable whirls were generally associated with flame heights smaller than the wall height of the square enclosure. Flame temperatures were primarily affected by the magnitude of the volumetric heat source.

Murgai and Emmons (1960) and Emmons and Ying (1966) describe integral plume models, which are calibrated with experimental data. Satoh and Yang (2000a) used the UNDSAFE code with associated 3d, compressible, buoyant, and constant turbulent viscosity specifications. Ten cases were considered which included validation exercises and parameter sensitivity studies.

Battaglia et al. (2000) simulated the laboratory experiments of Emmons and Ying (1966), Chigier et al. (1970), and Satoh and Yang (1997), which included cases for fixed circulation and variable fire strength, fixed fire strength and variable circulation, and jointly varied fire strength and circulation. The numerical code used was the NIST shareware FDS (Fire Dynamics Simulator) which includes 3d, compressible, buoyant and LES turbulent models (Baum et al., 1996).

Meroney (2001, 2003, 2004) considered the growth of fire whirls in large building atria and their effects on distribution of smoke and building evacuation. Using the commercial CFD code, FLUENT, he reproduced the transient growth and stabilization of laboratory fire whirl configurations used by Byram and Martin (1962), Emmons and Ying (1966) and Satoh and Yang (1997) to verify the codes suitability for fire whirl research.

Laboratory tests from Byram and Martin (1970) and Satoh and Yang (2000a) were reproduced with FLUENT to study the dominant features of fire whirl kinematics and to verify the codes suitability for fire whirl research. The Byram and Martin laboratory configuration consists of a cylindrical shell 66 cm diameter and 183 cm high over which is mounted a truncated conical shell 152 cm high that tapers from a base of 66 cm diameter to a top of 33 cm diameter. Air enters the chamber through two 0.6 cm tangential slits located on opposite sides of the cylindrical section, producing rotation of the air inside. The heat source is a 11.4 cm

diameter pool of burning alcohol located at the cylinder base at the central axis which releases about 11,600 watts of energy.

The numerical domain was configured with similar dimensions, included 75,604 hexagonal cells, and imposed a 11.6 kW heat source at the chamber base. The rising flame produced within the cylindrical enclosure five seconds after ignition initially rose vertically in a tall thin column, after 9 seconds it fell back and slowly rotated about the pan, and then it rose vertically again and stretched upwards. During the experiment the scientists also found “As the heated air rises and cool air flows tangentially into the chamber, the flame tilts in the form of a curved arm which slowly rotates around the pan” (Byram and Martin, 1970). Eventually the flame curls back on itself and begins to spiral upward, but, as noted by Byram and Martin, “This wander appeared to be caused by some inherent instability of the fire whirl, since 6 months of effort failed to find any external cause.” Subsequently, the fire whirl lengthens stretches and rises along the chamber axis in a tube-like column.

To replicate the Satoh and Yang experiments, a rectangular chamber was formed from finite height vertical walls 180 cm tall rising around a 63 cm square courtyard with four 12 cm wide gaps extending along each corner. The chamber resided within a 1m x 1m x 2m computational domain that included 22,300 tetrahedral cells. In this case the heat source was presumed to be a vertical volume centered over a 21 cm square fire pan extending 90 cm tall. 20 kW of heat were released throughout the flame volume at rates varying from 0.3 to 1.9 MW/cubic meter to replicate the behavior of burning heptanes as suggested by Satoh and Yang (2000a). Again the rising flame produced within the rectangular enclosure rose vertically during the initial flame development period from 0 to 10 seconds. Next, down flow from the top caused the flame to tilt over and revolve around the burner in the form of a nearly horizontal arm of flame, which precessed about the chamber every 3 seconds. After about 30 seconds the flame stabilized itself and began to stand upright and elongate. By 40 seconds the vortices coalesced into a single spiral fire whirl column. The sequence of events and flow characteristics observed during the numerical simulation are in the same order, occur at similar times and have the same magnitudes as observed by the experimenters.

Given that the CFD model reproduced fire whirl kinematics observed during different laboratory experiments, it was felt reasonable to perform sensitivity studies to determine what ventilation and exhaust geometries might produce fire whirls at building atria scales (Meroney, 2001, 2003).

5.0 SUMMARY OF LIMITATIONS OF METHODOLOGY AND RESEARCH NEEDS

Good mental health in a fluid or CFD modeler is always indicated by the presence of a suspicious nature, cynicism and a “show me” attitude. These are not necessarily the best traits for a life mate or a best friend, but they are essential if the integrity of the modeling process is to be maintained.

5.1 *Limitations of Similitude*

It is important to remember that models are “virtual” reality and only as accurate or realistic as our own imagination. When we insist on modeling at reduced length scale ratios simulation criteria often require metrology decisions that may enhance one flow characteristic while degrading another. We will never fully be able to answer the question “*Just how reliable are the results?*” Simulation must be limited by uncertainties in our understanding of the physical phenomena, uncertainties about the initial or boundary conditions, uncertainties about our measuring equipment, uncertainties about our prototype observations, and uncertainty about what we really want to know.

We must also take care that our search for agreement and correlation does not itself lead to “*spurious*” errors and self-deception (Meroney 1998b). Data presentation suggested by scaling variables and simulation criteria might itself misrepresent the results. Flawed analysis either intentional or through misunderstanding of commonly accepted data analysis methods can lead to erroneous results and presumption of correlation of cause and effect, when, in fact, there is little or none. Classical dimensional analysis combined with statistical regression of such scaled data may produce apparent correlation of information resulting in “virtual” or “spurious” correlation. Such inadvertent correlation errors can result in inappropriate conclusions and self-deception concerning the actual relationships between scaling variables and the associated reduction in variance found in tables and graphs. A number of dimensionless expressions used in meteorology and wind engineering induce large magnitudes of spurious correlation when plotted against other commonly accepted parameters. For example, when drag coefficients, C_D , pressure coefficients, C_p , dimensionless shear, S^* , or dimensionless concentrations, K , are regressed against Reynolds numbers, Re , dimensionless height, z/L_{MO} , or stratified Jensen numbers, z_0/L_{MO} , inherent virtual correlations can exist with values from 50 to 95% even when random numbers are used to generate the component parts of the dimensionless groups!

Despite the limitations noted above, careful fluid modeling is often still the best and only reliable predictive tool available! Every caution that can be applied to fluid modeling must also be applied to analytic and numerical modeling.

5.2 *Specific Modeling Limitations Yet Unresolved*

Sometimes fluid and numerical model capacity is limited by our own limited understanding of the fluid phenomena. For example, better simulations await the ability to provide:

- Consistent inlet flow during CFD simulation of scales and characteristics of the atmospheric boundary layer (reproduction simultaneously of U, I, and L profiles which are in equilibrium).
- Simultaneous resolution of small and large scales (e.g. fire involves scales from microns to km).
- Simultaneous similitude when conflicting similarity requirements exist (e.g. Fr and Re number, one requires U proportional to L and the other $L^{1/2}$).
- Turbulence models that correctly model the balance of turbulent production and dissipation (e.g. standard kappa-epsilon model presumes equilibrium in production and destruction of turbulence energy in situations where significant convection is actually present, but large eddy simulation models are known to incorrectly model jet growth rates if incorrect constants are chosen).
- Chemical reaction models that do not impose reaction time scales which are incompatible with other fluid modeling similitude requirements.
- Sensitivity studies which define model sensitivities (e.g. Beychok (2004) notes that uncertainties in input information can propagate through analytic models for plume rise, dispersion coefficients and concentration averaging to produce potential errors by factors of six to eighty).

5.3 *Air Pollution Aerodynamics in the 21st Century*

The primary role of fluid modeling of air pollution aerodynamics during the next century will not always be the direct measurement of data to be used during engineering design of specific facilities. Fluid modeling is often not fast or flexible enough to perform the sensitivity studies

commonly required making engineering decisions about very complex systems. Instead fluid modeling should be used:

- To explore atmospheric dispersion interactions not yet fully understood,
- To tune and justify turbulence models incorporated into CFD models,
- To complement (or replace) numerical measurements when the veracity of CFD modeling is constrained by computational capacity, understanding, or economics,
- To devise new analytic models suitable for inclusion in larger numerical systems, and
- To validate computational modules as they are incorporated into computer design codes.
- To assist in the “education” of a new generation in fluid dynamics and wind engineering.

The proliferation of conference titles and sessions focusing on CFD and wind engineering suggests that this refocus is already underway.

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Following figures provided by Chris Rahaim, Co-Chair of AIAA Committee on Standards for Computational Fluid Dynamics, September 2004.

The Scientific Method as Practiced Before Digital Computers

- Practiced by Hippocrates (460-377 BC), In His Rational, Empirical Approach to Medical Science
- Described and Practiced by Descartes (1596-1650)
- Established On Two Foundations:
 - Experimental Science
 - Theoretical Science
- Characterized by Continuous Process of Improvement and Discovery
- Data Validation Process
 - Units of Measurement, Datums
 - Error and Uncertainty Quantification

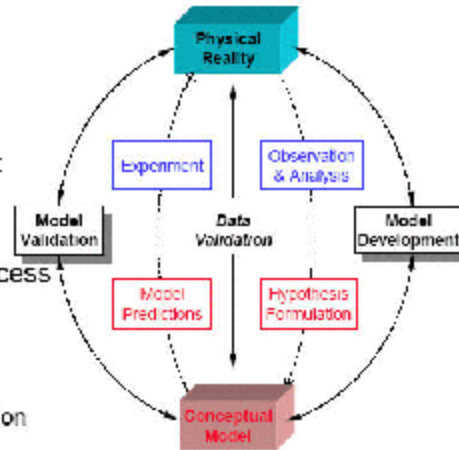


Figure 1 The “Old” Scientific Method. Cosner and Rahaim (2001), QNET-CFD Conference, Athens, Greece, May 2001.

The “New” Scientific Method (Based on Sargent’s Framework)

- Supported by Three Foundations:
 - Experimental Science
 - Theoretical Science
 - Computational Science
- The Processes of Model Development, Verification, and Validation Deal Respectively, with the Interfaces Between:
 - Reality - Model
 - Model - Simulation
 - Simulation - Reality

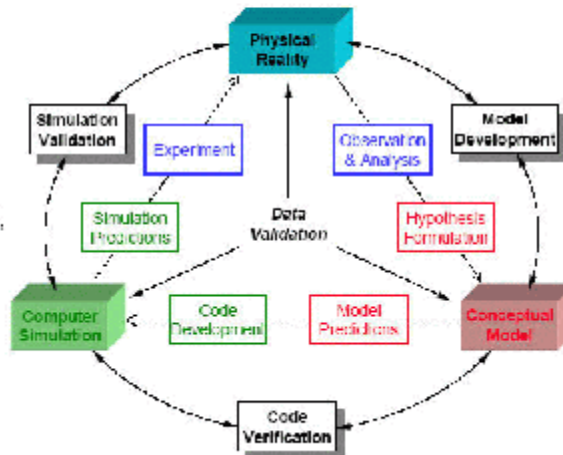


Figure 2 The “New” Scientific Method. Cosner and Rahaim (2001), QNET-CFD Conference, Athens, Greece, May 2001.