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Validation Data for Models of Contaminant Dispersal: Scaling Laws and Data Needs

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Validation Data for Models of Contaminant Dispersal: Scaling Laws and Data Needs

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ABSTRACT

Contaminant dispersal models for use at scales ranging from meters to miles are widely used for planning sensor locations, first-responder actions for release scenarios, etc. and are constantly being improved. Applications range from urban contaminant dispersal to locating buried targets from an exhaust signature. However, these models need detailed data for model improvement and validation. A small Sandia National Laboratories Laboratory Directed Research and Development (LDRD) program was funded in FY04 to examine the feasibility and usefulness of a scale-model capability for quantitative characterization of flow and contaminant dispersal in complex environments. This report summarizes the work performed in that LDRD. The basics of atmospheric dispersion and dispersion modeling are reviewed. We examine the need for model scale data, and the capability of existing model test methods. Currently, both full-scale and model scale experiments are performed in order to collect validation data for numerical models. Full-scale experiments are expensive, are difficult to repeat, and usually produce relatively sparse data fields. Model scale tests often employ wind tunnels, and the data collected is, in many cases, derived from single point measurements. We review the scaling assumptions and methods that are used to relate model and full scale flows. In particular, we examine how liquid flows may be used to examine the process of atmospheric dispersion. The scaling between liquid and gas flows is presented. Use of liquid as the test fluid has some advantages in terms of achieving fully turbulent Reynolds numbers and in seeding the flow with neutrally buoyant tracer particles. In general, using a liquid flow instead of a gas flow somewhat simplifies the use of full field diagnostics, such as Particle Image Velocimetry and Laser Induced Fluorescence. It is also possible to create stratified flows through mixtures of fluids (e.g., water, alcohol, and brine). Lastly, we describe our plan to create a small prototype water flume for the modeling of stratified atmospheric flows around complex objects. The incoming velocity profile could be

tailored to produce a realistic atmospheric boundary layer for flow-in-urban-canyon measurements. The water tunnel would allow control of stratification to produce, for example, stable and unstable atmospheric conditions. Models ranging from a few buildings to cityscapes would be used as the test section. Existing noninvasive diagnostics would be applied, including particle image velocimetry for detailed full-field velocity measurement, and laser induced fluorescence for noninvasive concentration measurement. This scale-model facility will also be used as a test-bed for data acquisition and model testing related to the inverse problem, i.e., determination of source location from distributed, sparse measurement locations. In these experiments the velocity field would again be measured and data from single or multiple concentration monitors would be used to locate the continuous or transient source.

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ACKNOWLEDGMENTS

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EXECUTIVE SUMMARY

Contaminant dispersal models are widely used for planning sensor locations, first-responder actions for release scenarios, etc. and are constantly being improved for applications ranging from urban contaminant dispersal to locating buried targets from an exhaust signature. Detailed data sets are needed to improve models and to validate contaminant dispersal simulations. This report summarizes the data needs for model improvement and validation and demonstrates the physical scaling laws that allow a "real-world" release to be experimentally simulated in a laboratory-scale facility. A small Sandia National Laboratories Laboratory Directed Research and Development (LDRD) program was funded in FY04 to examine the feasibility and usefulness of a scale-model capability for quantitative characterization of flow and contaminant dispersal in complex environments. This report provides justification for use of scale-model experiments and for the use of water instead of air as the working fluid. Results of discussions with atmospheric dispersion model developers and users are included. Finally, the proposed experimental testbed is described. The testbed would be configurable to simulate flow in a city or in a cluster of buildings. It would most likely be a water tunnel or flume where the incoming velocity profile could be tailored to produce a realistic atmospheric boundary layer for flow-in-urban-canyon measurements. The water tunnel would allow control of stratification to produce, for example, stable or unstable atmospheric conditions. Existing noninvasive diagnostics would be applied, including particle image velocimetry for detailed full-field velocity measurement, and laser induced fluorescence for noninvasive concentration measurement. Discrete concentration monitors would be used for point concentration measurements and for "bird-dog" experiments testing source identification algorithms.

INTRODUCTION

The threat of accidental or intentional release of chemical, biological, and radiological agents and contaminants is increasingly of concern. As such, civil defense and military planners are now being asked to assess the potential risks associated with a release. Planners would like to know what steps can be taken *before* any release to reduce the potential harm that might occur. They need to predict the *extent*, *duration* and *level* of contamination given the large variety of possible release methods and agents. And, they need to *assess* the consequences of any actual releases both in near real time and during post-event analysis.

It is impractical to experimentally examine all the possible release scenarios. Consequently, a variety of atmospheric dispersion models have been developed over the years to aid in the prediction of atmospheric contaminant dispersion. Both civilian and government scientific and engineering organizations have created and used atmospheric dispersion models to track the dispersion of pollutants, plumes resulting from building or forest fires, weapons fallout, and naturally occurring emissions such as volcanic eruptions, among many other applications. Military uses have included tracking plumes from burning Kuwaiti oil fields and chemical weapon demolition during the first Gulf War (Gamboa, 2003).

A significant number of dispersion models have been developed. A workshop on atmospheric dispersion modeling within the federal community in the year 2000 identified 64 dispersion models used by federal agencies ranging including DoD, DoE, NOAA, EPA, USDA, USGS, DoT, FEMA, NIST, NASA, and DTRA (Harrison, 2000). The National Research Council published an overview of the field in 2003 entitled "Tracking and Predicting the Atmospheric

Dispersion of Hazardous Material Releases - Implications for Homeland Security" (hereafter referred to as the AD-NRC report). That report summarizes both the needs for, and current capabilities of, atmospheric dispersion modeling and experiments. Eleven dispersion models were identified and discussed. The large number of models points to the variety of modeling assumptions employed and the differing flows and types of contaminant releases under consideration.

The length and time scales of the atmospheric flows are broadly classified in **Table 1**.

Scale	Length Scales	Time Scales
Street Scale (Local)	100 m or less	Seconds to Hours
Neighborhood (Local)	100 m to1 km	Minutes to Hours
Microscale or City Scale (Urban and County)	1 km to 10 km	Minutes to Hours
Mesoscale or Regional Scale (State and Region)	10 km to 1000 km	Hours to Days
Continental and Global	Greater than 1000 km	Days

Table 1: Classification of the scales in the atmosphere.

The modeling assumptions and methods will differ depending upon the scale of the flow under consideration. First, the underlying atmospheric boundary layer flow must be computed, including mass, momentum, and heat transfer processes. Next, the process of contaminant release and dispersion must be modeled and coupled to the flow.

The atmospheric boundary layer (ABL) comprises the lower one to two kilometers of the atmosphere which is strongly affected by the surface conditions and surface heating and cooling. The ABL itself has a wide range of flow scales, is generally turbulent, and often has stratification of temperature and density. The ABL can be divided into several layers, with the layer closest to the surface being the surface layer composed of the "roughness layer" with thickness on the order of 10 m, and the "inertial sublayer" with thickness of order 100 m. The roughness sublayer in an urban setting is typically approximately twice the average building height (Britter and Hanna, 2003). The surface layer is a layer of approximately constant shear stress (Fernando et al., 2001). The "outer" (Ekman) layer has a thickness on the order of 1 km. **Figure 1** shows a schematic drawing of the flow over an urban canopy. The ABL velocity profile is complicated by atmospheric stability conditions but in general the flow in the surface layer, above the roughness layer and under conditions of neutral stability, shows an overall logarithmic increase of mean horizontal velocity $\bar{u}$ with height z which can be expressed as:

$$\bar{u} = \frac{u^*}{\kappa} \ln\left(\frac{z-d}{z_0}\right) \tag{1}$$

where u* is the friction velocity determined by the surface shear stress, κ is the von Karman constant (κ ≈ 0.40), z_o is the roughness length scale, and d is the boundary layer displacement caused by the presence of the roughness elements. Typical values of the roughness length scale range from 0.1 m for open country to 2.0 m for "chaotic" city centers (Britter and Hanna, 2003). The overall logarithmic profile is similar to the aerodynamic boundary layer over a rough surface. Note that this is a simplified view of the flow over a rough surface. Details like a thin viscous sublayer are not shown, but such effects are negligible or nonexistent in a turbulent ABL flow over a rough surface (Garratt, 1992; Sorbjan, 1989).

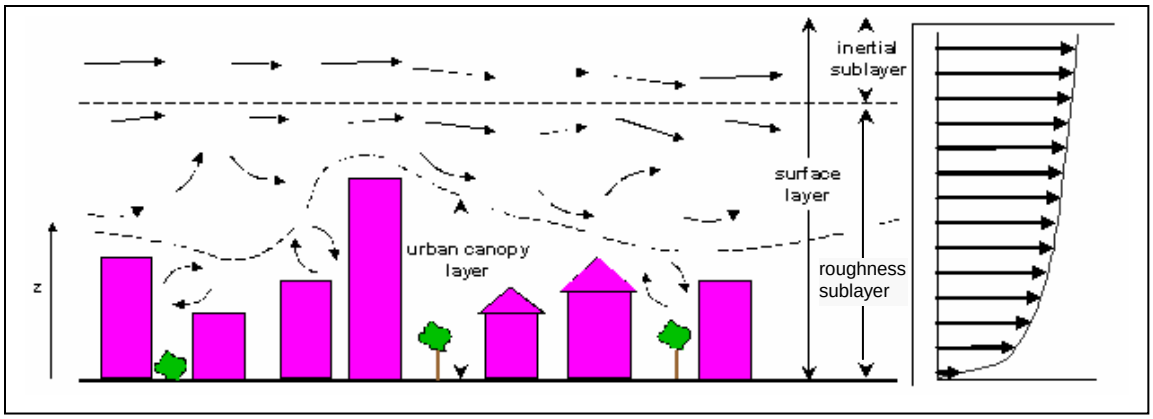

Figure 1: Schematic of the atmospheric boundary layer flow over an urban canopy (based on Britter and Hanna, 2003).

The heating and cooling of the earth's surface that occur during the diurnal cycle can lead to stratification of the atmospheric boundary layer. **Figure 2** shows a typical 24 hour cycle. Surface heating during daylight hours leads to a convective boundary layer that grows during the day. Atmospheric boundary layers can be classified as "neutral" when buoyancy effects are small. This might occur when it is a windy day with cloud cover. A "convective" boundary layer occurs when surface heating leads to unstable density stratification and thus to strong convective flows. During nighttime, a stable "nocturnal" boundary layer may form near the ground as heat is radiated away from the surface and the air is cooled. The presence of stratification can have significant influence on the process of contaminant dispersion.

Monin-Obuhkov similarity (Garratt, 1992) is based on the Monin-Obuhkov length scale L_{MO} which is the height at which the shear and buoyancy terms of the turbulent kinetic energy transport equation become equal. In other words, at the height L_{MO} the work done by Reynolds stresses is balanced by that done by surface heating (buoyancy). Positive values of L_{MO} indicate stable stratification, negative values indicate unstable (convective) stratification, and L_{MO} is infinite for neutral stratification.

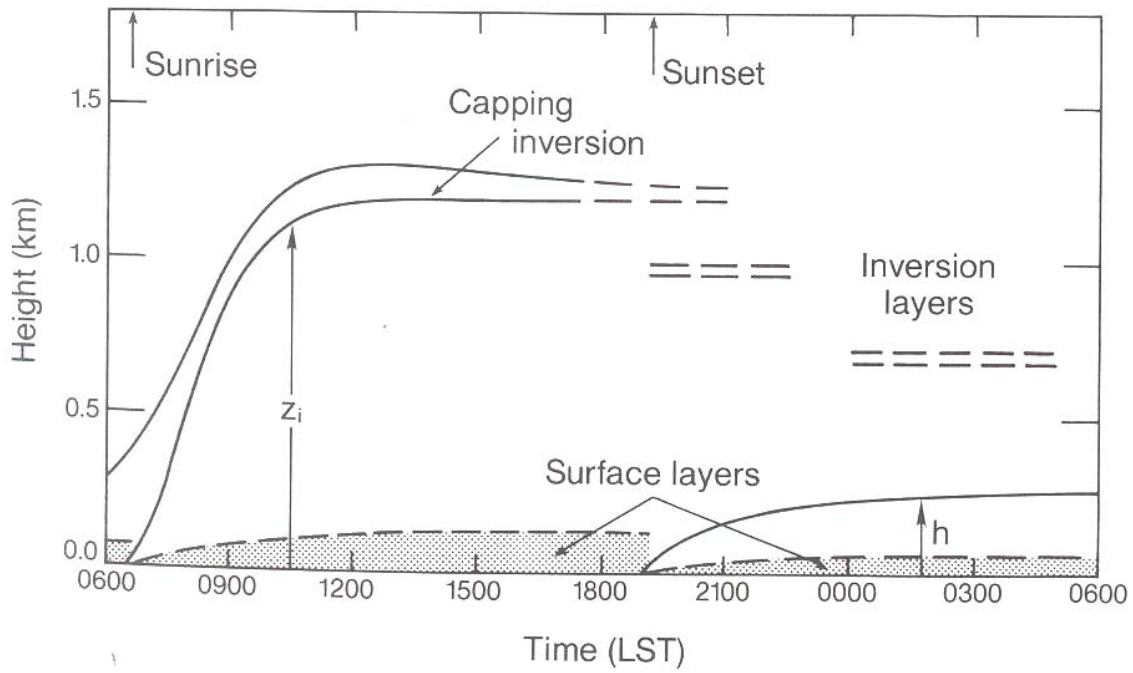

Figure 2: The diurnal cycle of the atmospheric boundary layer over land (Garratt, 1992)

Dispersion models can be organized by the complexity and fidelity of the underlying transport models. Many models will compute only the *average* properties of the flow, including average flow directions and temperature, turbulence levels, and contaminant concentrations. Simplified models of dispersion have been used for some time whereby the average wind direction and turbulence level is used to predict the rate of plume convection and entrainment. These schemes are often referred to as *Gaussian Plume* models, with the most common being the Pasquill-Gifford model (Stull, 2000). Gaussian plume models can quickly yield an estimate of the time-averaged location and concentration of the contaminant plume. Such data can be useful for first responders (Brown and Streit, 1998).

More complex models attempt to compute the spatially- and time-resolved flow fields. Because of the large range of scales in the atmospheric boundary layer dispersion problem, it is not possible to compute the flow field from direct numerical solution of the underlying conservation equations (i.e., direct numerical simulation). Rather, only a range of large flow scales is resolved, while the physical processes within the unresolved scales are modeled. These types of models are often referred to as *Large Eddy Simulation* (LES) models. LES models can be used to produce both time-averaged and temporally-resolved predictions of the contaminant location and concentration. As the range of the resolved scales increases, the computational resources necessary to compute the flow field increase dramatically. Thus, the significant improvement in predictive capability that LES provides comes with the cost of significant time and effort needed for the computations.

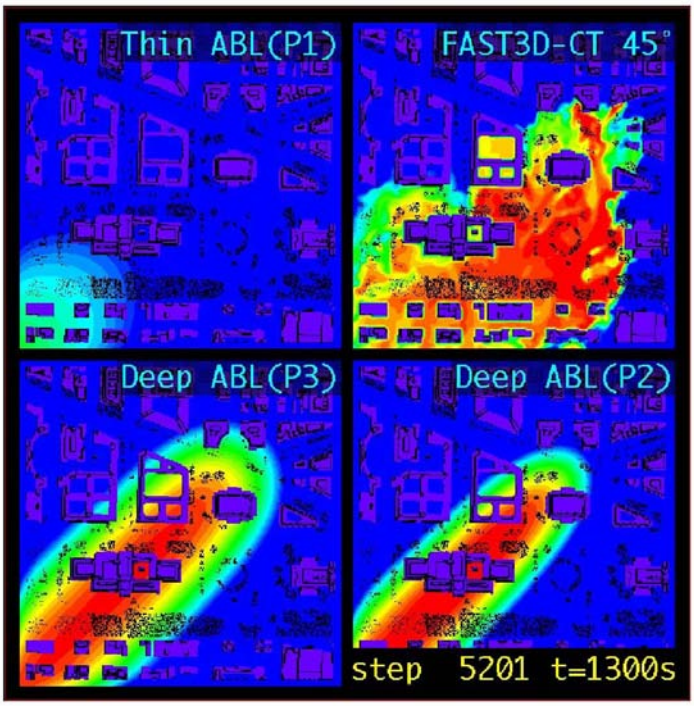

Figure 3: A comparison between LES and Gaussian Plume models for simulation of the release of a contaminant in an urban canopy, (Boris, 2004)

Figure 3 shows an example simulation of a plume release simulated with the LES-based dispersion model FAST3D-CT along with three possible Gaussian plume computations. In each case the point source was located on the ground 500 meters upwind of the target building and the wind was from the northeast at 3 m/s. Each of the plume solutions used a stratified boundary layer velocity profile with different scale heights. The run "P1" used a roughness length z_o = 10 cm, characteristic of the atmospheric boundary layer over an open area, as input to many Lagrangian puff models. "P2" used z_o = 30 cm, a deeper boundary layer, and "P3" used the urban boundary layer as determined by FAST3D-CT simulations. The diffusive transport coefficients give representative plume widths. Note that the Gaussian plume solutions (P1, P2, and P3) do not capture the shape, building wake trapping behavior, or plume width predicted with the LES model (Boris, 2002, 2004). Of course the plume models do not model the buildings as in FAST3D-CT, where the buildings are included in the computational mesh. Therefore the Gaussian plume models (P1 – P3) cannot be expected capture any of the building effects.

It is important to consider what the desired product of the dispersion model actually is. One may wish to determine the *average* level of a dispersed contaminant that will occur at any particular location in the vicinity of a release. Or, one may wish to know the *peak or range* of possible contamination levels that may be realized. Average quantities may be sufficient to describe the dispersion field if the release is steady and from a fixed location (such as an industrial smoke stack). However, if the release is transient and the source complex, it may be much less useful to consider only time-averaged quantities. The inherent variability in the atmospheric boundary flows adds to the complexity of predicting transient dispersion events. Users of dispersion models must therefore determine the level of model complexity and fidelity necessary to achieve their goals.

A significant distinction can also be made between dispersion modeling of city scale flows compared to the neighborhood and street scales. In the former, the topology of buildings and trees are considered as an average degree of surface roughness elements beneath the turbulent atmospheric boundary layer. The detailed flow within the urban canopy is not considered. However, in the neighborhood and street scales, the complex flow within the urban canopy governs the dispersion process (Fernando et al., 2001; Britter and Hanna, 2003). The detailed processes of near-surface heat transfer and mechanical flow forcing (e.g., the motion of vehicles) can also significantly influence the dispersion processes. While a significant amount of effort has been devoted to developing dispersion models for city scales and greater, the complex process of dispersion in the urban canopy has not received the same degree of study. Britter and Hanna (2003) stated the following conclusions in their recent review of urban dispersion processes:

> "In a fluid-mechanical context, the most pressing problems include the treatment of atmospheric stability in urban areas, the specification of reference variables (e.g., the wind speed well above the urban area, the wind speed just above or at the average building height, and the wind speed within the urban canopy), and the treatment of arbitrary spatial variations in roughness."
>
> "For dispersion studies it is still unclear how best to address the neighborhood scale and its connections with the street and city scale, especially when addressing transient problems."

Thus, tracking of airborne contaminants that result from transient releases in a complex flow environment presents a challenging problem for modelers.

FULL SCALE EXPERIMENTAL DATA FOR MODEL VALIDATION

Before any model can be used, it must first be validated. Ideally, controlled experiments are conducted and the results compared with the prediction of the model. While many attempts to validate atmospheric dispersion models have been conducted over the years, the results are often difficult to interpret. This problem is discussed in the AD-NRC report. Consider the continuous release from a point source. The effluent concentration can be measured at a given downstream location to determine the average value. **Figure 4** illustrates how the instantaneous value of the concentration can vary widely since the dispersion cloud is not a steady plume but may have complex vortical structure, and the plume may meander under the influence of the prevailing winds. If the winds are unsteady, it may take as long as several hours for a statistically stationary average to be obtained.

Long-time averages are not appropriate in the case of transient releases. Instead, a prediction of the *time dependent probability* of the plume concentration is needed. This is a much more challenging task, and such models are only recently being considered. To validate such probabilistic models, a large number of experiments and simulations may need to be performed. Repeated full-scale experiments are difficult to achieve since the environmental boundary conditions during the experiments must also be considered in establishing repeatability. This is especially true for full-scale or field validation experiments. **Figure 5** illustrates some of these differences for full-scale and wind-tunnel flows, and the flows predicted by Gaussian plume models.

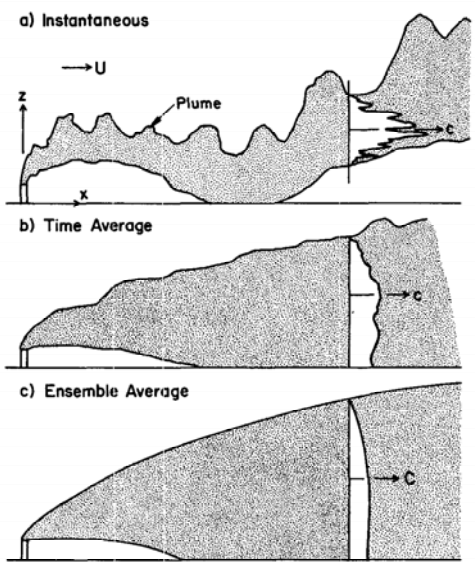

Figure 4: Schematic diagram showing the instantaneous, time averaged, and ensemble average concentration profiles downstream of a smokestack (Weil et al., 1992).

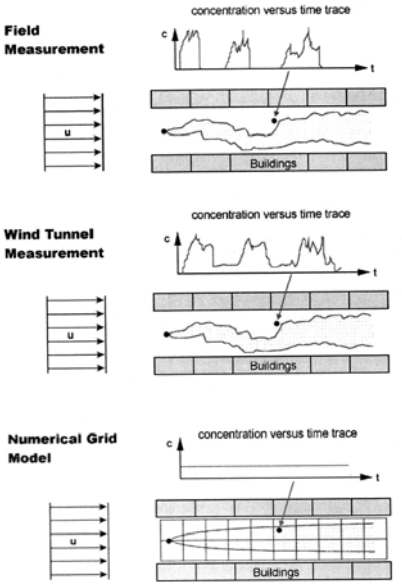

Fig. 1. Comparison of concentration versus time traces typical for field measurements (top), wind tunnel measurements (centre) and numerical model results (bottom) (concentrations in excess above ambient only).

Figure 5: Schematic diagram showing the differences between field, wind tunnel, and a Gaussian plume prediction for flows between buildings (Schatzman and Leitl, 2002).

Ultimately, when the experimental data are compared with model predictions, the variability inherent in the experiment due to changing atmospheric conditions must be characterized. Otherwise, it will not be possible to determine if discrepancies between model predictions and the experimental data result from modeling limitations. **Figure 6** shows data presented by Weil et al. (1997) for the dispersion of an industrial pollutant. A comparison is made between experimental observations and the predictions of a Gaussian plume model. Note the large number of finite concentrations measured when zero concentration was predicted. This resulted from the instantaneous wandering of the plume into a region where the Gaussian plume model predicted a very low *average* concentration. The significant scatter in the data results from a combination of variability in environmental flow conditions, uncertainty in the model input parameters, and limitations in the physical model itself.

Thus, one challenge of conducting full-scale tests is to collect enough data about the underlying atmospheric flow in order to fairly evaluate the model. A variety of instruments and methods are used to record such environmental quantities as wind speed and direction, atmospheric turbulence, atmospheric temperature and stratification, humidity, and effluent concentration. Some measurements provide data at discrete locations (e.g., wind gauges and thermometers), while other sensors can provide data fields (e.g., RADAR, LIDAR, and satellite imaging). Usually a combination of sensors is used to produce as complete a data set as possible given the constraints of time and resources. In general, the cost and complexity of full-scale testing limits the number of tests that can be performed. Despite such well-understood and commonly acknowledged limitations, the need for good validation data has led to a series of full-scale and outdoor experiments. Recent examples are listed in Table 2.

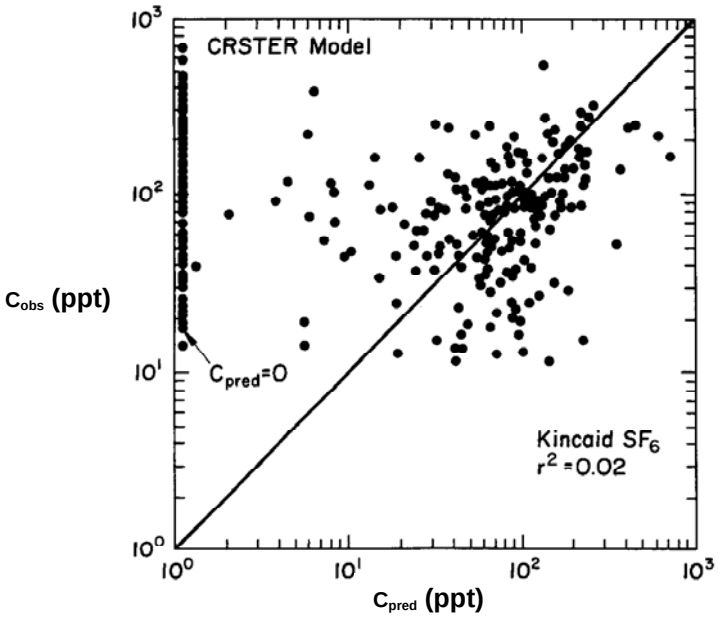

Figure 6: The comparison between the predicted and measured plume concentrations reported by Weil et al. (1997). The predictions were made with a Gaussian plume model.

Experiment	Organizer	Date	Location	Measurements	Number of Runs
Urban 2000 (http://urban.llnl.gov/)	LLNL	October 2000	Salt Lake City, Utah	Temperature (29 + 1 mobile) Sonic Anemometers (14-2D and 9-3D) LIDAR (2) RADAR SODAR (3) Energy Budget Station (1) SF_6 and PFT Tracers > 15 Trace Samplers	Runs over 7 days
Kit Fox (Hanna and Steinbring, 2001; Hanna and Chang, 2001)	Petroleum Environmental Research Forum	September 1995	French-man Flat, Nevada	Uniform Roughness Array and scale models CO_2 Tracer Fast Response Tracer samplers (84) Sonic Anemometers (10)	52 trials
Joint Urban 2003 (http://ju2003.pnl.gov/) Allwine et al., 2004.	DoE, DoD, DHS, UK-DSTL	July 2003	Oklahoma City, Oklahoma	Wind Stations (~200) Tracers Samples (>200)	10 trials
Bubble 1 (http://www.unibas.ch/geo/mcr/Projects/BUBBLE) Gryning et al, 2003; Christen et al., 2002.	Swiss Ministry of Education and Science	Summer 2002	Basel, Switzer-land	wind profiler, SODAR, RASS and LIDAR), SF_6 tracers	Full year atmospheric data, SF_6 during portion

Table 2: Some recent outdoor dispersion experiments

The Urban 2000 and the Joint Urban 2003 (**Figure 7** and **Figure 8**) studies were used to examine dispersion in the urban canopy along with the intrusion of contaminants into building ventilation systems. The Kit Fox experiments were a series of outdoor experiments designed to examine flows over 1/10 scale models of an industrial site. The data from these tests are used to develop and validate models. The planning and execution of these trials involves considerable effort and expense. In some instances, model scale tests are conducted to aid in the planning of large-scale trials and to support interpretation of the resulting trial data.

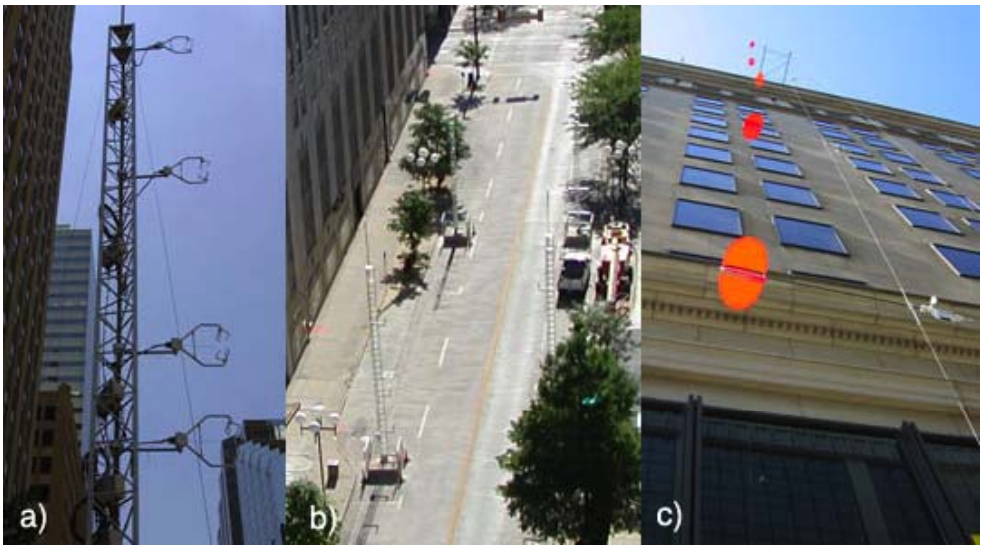

Figure 7: Images of wind speed measurement devices deployed in Oklahoma City during the Joint Urban 2003 full-scale dispersion experiment (Brown et al., 2004).

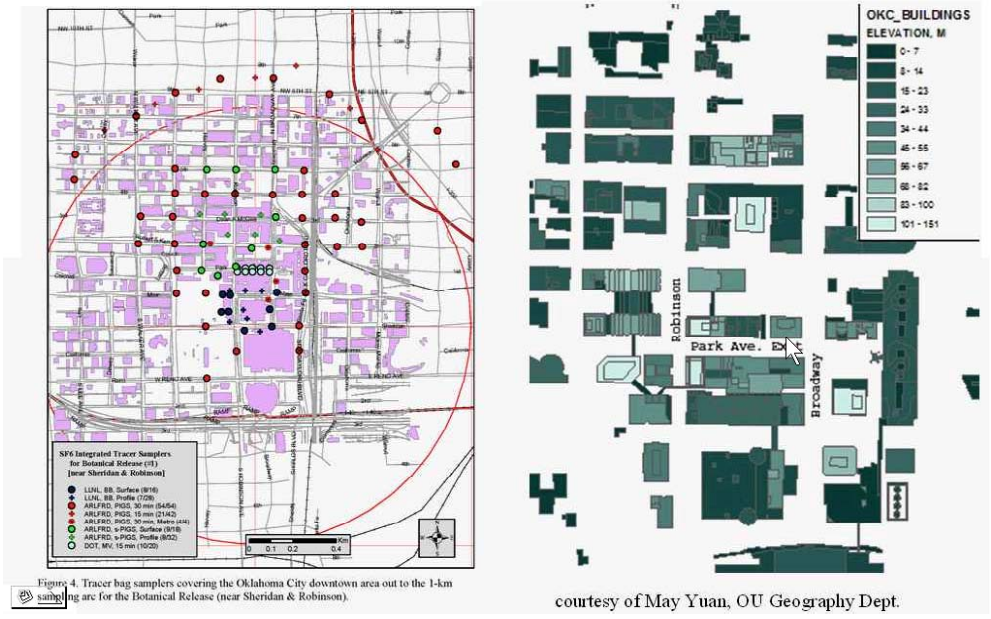

Figure 8: A map of sensor location placed in Oklahoma City during the Joint Urban 2003 full-scale dispersion experiment (Brown et al., 2004).

MODEL SCALE EXPERIMENTAL DATA FOR MODEL VALIDATION

Model testing of dispersion processes provides an alternative to full-scale validation experiments. Wind tunnel testing has been extensively used for wind engineering, with scale models of buildings and structures often being tested for both static and dynamic wind loads. Wind tunnel testing has also been used to study the dispersion of contaminants. Physical scale factors are generally 1:100 to 1:1000. Specially modified wind tunnels used for such experiments are often referred to as Meteorological Wind Tunnels. **Table 3** presents a list of some meteorological wind tunnels currently used for dispersion studies.

Owner	Location	Test Section Size	Maximum Speed	Special Features
Colorado State University	Fort Collins, CO	1.8 m x1.8 m x 26.8 m	To 37 m/s fps	Humidity Control; Heated/Cooled Floor
US -EPA	Research Triangle Park, NC	3.7 m x 2.1 m x 18.3 m	0.3 to 8 m/s	
University of Surrey	Guildford, UK	1.5m x 3.5 m x 27 m	0.3 to 4.5 m/s	Heated/Cooled air and surfaces
Arkansas Chemical Hazards Research Center	Fayetteville, AR	2.1 m x 6.1 m x 24.4 m	Minimum speed 0.2 m/s	
University of Hamburg	Hamburg, Germany	8m long, 4m wide with an adjustable ceiling height of 2.75 - 3.25 m		

Table 3: A list of some meteorological wind tunnels used for dispersion studies.

Meteorological wind tunnels differ from conventional aerodynamic wind tunnels in several ways. First, the test section of a meteorological wind tunnel is typically longer to permit the generation of a scaled atmospheric boundary layer before the flow reaches the test model, although not so long that natural boundary layer development can be used to form a scaled atmospheric boundary layer (Obasaju and Robins, 1998). Instead, boundary layer generators are used to create a scaled atmospheric boundary layer in a shorter fetch. Both tall, thin vortex generators ("spires") and surface roughness elements are used to produce an inlet mean and turbulent velocity profile. Second, some meteorological wind tunnels allow for heating and cooling of the inlet airflow and flow surface in order to generate non-neutral boundary layers. Third, the typical flow speeds needed for appropriate Reynolds number scaling are generally quite low. **Figure 9** shows two images of models in the test section of meteorological wind tunnels.

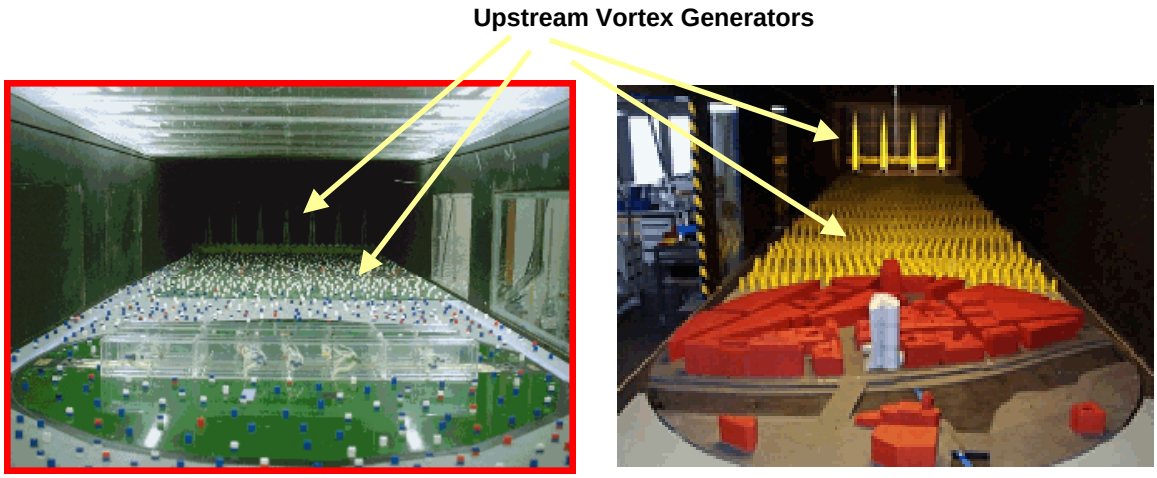

Figure 9: Images of the test section from scale model tests in two meteorological wind tunnels (http://weather.ou.edu/~pkklein/windtunnel/windtu.html#studies and http://www.gfa.de/en/wind_engineering/).

The use of wind tunnel testing for engineering and regulatory studies is well established (Obasaju and Robins, 1998). Often the goal of the study is to determine if the normal or accidental emission from an industrial facility meets regulatory guidelines. In such studies, a scale model is built for wind tunnel testing of dispersion around an approximately 1 km radius of the release. Neutral and sometimes stratified inlet boundary layers are produced. The typical average free-stream speed is between 1 and 3 m/s. A tracer contaminant is then released with either a steady or pulsating mass flow-rate. The average cloud dimensions of the resulting plume are measured along with the maximum downstream concentration. These data are then used with a Gaussian plume model to predict plume size and concentration further downstream. The detailed flow in a complex geometry is usually not examined. Researchers at the Chemical Hazards Research Center at the University of Arkansas have developed a very low speed wind tunnel for dense-gas dispersion studies (Havens et al., 2001) which has been applied for studies of quasi-line source carbon dioxide releases. Simultaneous velocity fields and point concentration data were acquired.

The influence of stratification of the dispersion of contaminants can be significant, and this has led to the development of stratified meteorological wind tunnels as discussed above. These tunnels are not common, and their operation presents some challenges. First, the heating and cooling of the airflow often requires a considerable heat flux, and the process of heating and cooling can often obstruct optical access to the flow field, making experimental measurements more difficult. Second, the level of stratification that can be achieved is limited by the heat flux as well as the resulting heat loss through the walls of the test section. **Figure 10** shows a schematic diagram of the stratified wind tunnel facility at the University of Surrey, UK (see http://vortex.mech.surrey.ac.uk/FRC/facilities/enflo.html#EnFlo_Tunnel). For these reasons, researchers have explored the use of *stratified water channels* to study entrainment and mixing in stratified boundary layers. Many of these facilities are located at universities and are relatively

small. The University of Surrey also operates a stratified water channel that has been used to study atmospheric mixing and dispersion. This water facility has a 1.2 m x 1 m x 12 m with a 2 m x 1.65 m carriage, carriage operation at 0.03 to 0.3 m/s, and the ability to stratify using pure water, brine, and/or temperature. A discussion of the relative merits of wind and water testing will be presented below.

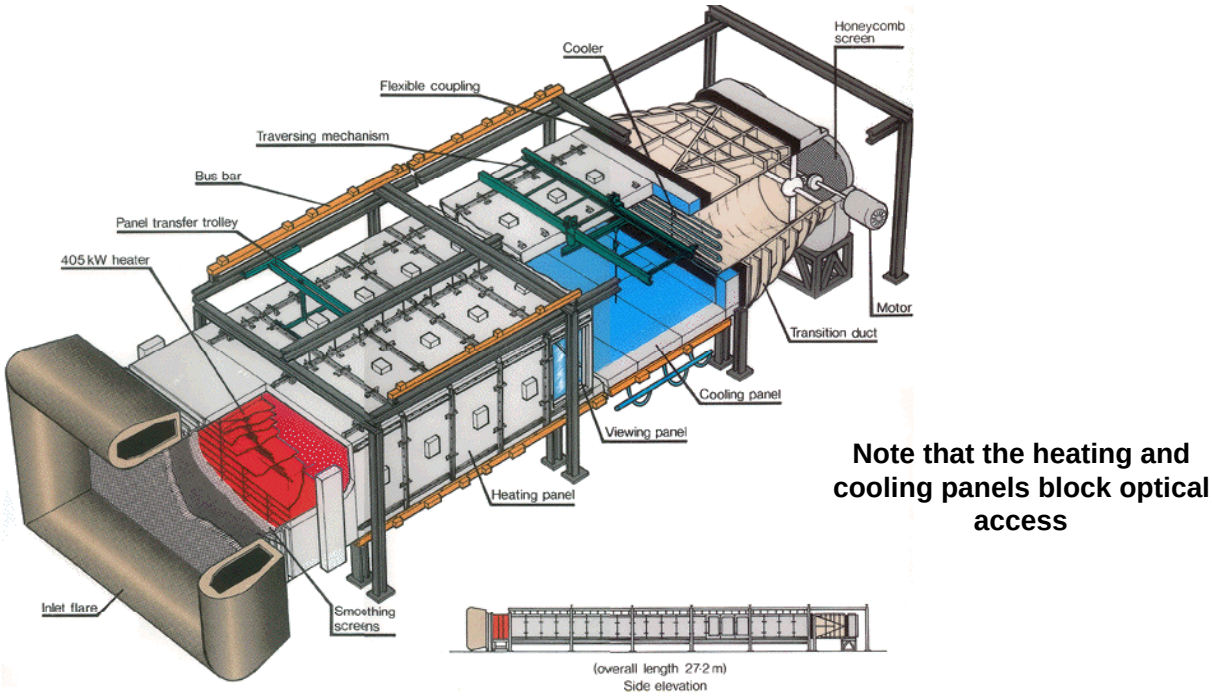

Figure 10: Schematic diagram of the stratified meteorological wind tunnel at the University of Surrey, UK. (see http://vortex.mech.surrey.ac.uk/FRC/facilities/enflo.html#EnFlo_Tunnel)

SCALING LAWS

Scale model testing in mechanical, aeronautical, and civil engineering has developed over the last 100 years. *Geometric*, *kinematic*, and *dynamic* similarity must be achieved between the model and full-scale flows in order to assure that the model results will represent the prototype conditions. This is accomplished through the appropriate identification of scaling parameters that must be compared between the model and full-scale realizations of the flow. It is usually not possible to exactly match every model and full-scale parameter, but model tests are still scaleable, even when the similarity is *incomplete*. The classic example involves the Reynolds number and dynamic similarity. The Reynolds number of a model scale aircraft might not exceed 10^6, while the actual prototype Reynolds number may be 100 times higher. Although the two parameters are not matched, the fact that they both exceed a critical value of 10^5 allows for the assumption of Reynolds number independence and, thus, dynamic similarity. For the case of airborne dispersion, the task is to identify which parameters are the most physically important, which must be matched between scales, and/or what critical values must be met for the remainder.

We are particularly interested in the comparison between air and water model testing in the case of airborne dispersion. Water flows have been used to model airflows for some time, and vice versa. For example, the U.S. Navy uses wind tunnel tests to examine the flows over submarine hulls, and water tunnel tests have been used to examine the flows around the body and under the hood of automobiles (e.g., Aroussi and Aghil, 2000).

There are many possible flow parameters that might be relevant to airborne dispersion. The most important parameters are discussed below.

Geometric similarity

The geometry of the model and full-scale flow boundaries must be similar. All pertinent features must be included in the scale model. In the case of airborne dispersion, the topology of the surface must be replicated. Usually the contour of the terrain is combined with models of tall buildings and other man-made flow features that are included in the scale model. The modeling of vegetation is often not included.

Reynolds number scaling

The primary dimensionless parameter that controls much fluid flow behavior is the Reynolds number, defined as:

$$\mathrm{Re} = \frac{\rho U L}{\mu} = \frac{U L}{\nu} \tag{2}$$

where ρ is the fluid density, U a characteristic fluid velocity, L a characteristic length scale, μ the fluid dynamic viscosity, and ν the fluid kinematic viscosity ($\nu = \mu/\rho$). The Reynolds number can be viewed as the ratio of inertial to viscous forces. Low Reynolds number flows are dominated by viscosity and are often laminar. High Reynolds number flows are generally turbulent.

Reynolds number scaling between a prototype or full-scale application and a scale model is best done by matching the Reynolds number of the two, for example:

$$\frac{U_p L_p}{\nu_p} = \frac{U_m L_m}{\nu_m} \tag{3}$$

where the subscripts "*p*" and "*m*" indicate "prototype" and "model", respectively. Reynolds number scaling can be used to determine the velocity at which a model experiment needs to be run in order to match full-scale flow conditions, as in:

$$U_m = \frac{L_p}{L_m}\frac{\nu_m}{\nu_p} U_p \tag{4}$$

In cases where the test fluids are known, thus fixing the ratio of kinematic viscosities, and the physical scale is known, thus fixing the ratio of length scales, Equation 4 gives the velocity at which to run the model experiment for Reynolds number matching of the full-scale application. However, as mentioned above, it is usually not necessary to exactly match the full and model scale Reynolds numbers. Instead, the model test must be conducted at a Reynolds number that exceeds a critical value. In the case of dispersion studies, the critical Reynolds number is ~1500. Flows at this Reynolds number are turbulent and the flow past bluff objects exhibits separation. For more streamlined or circular shapes separation will be delayed and the critical Reynolds number will be higher than that for bluff bodies. Consequently, a *minimum* Reynolds number is

usually prescribed for model tests. Model Reynolds numbers in excess of the critical Reynolds number are preferable, as the range of turbulent length scales (the turbulence cascade) increases with increasing Reynolds number (Finlayson et al., 2004).

For wind tunnel tests, the flow speeds needed to exceed the critical Reynolds are on the order of a few meters per second. This explains why meteorological wind tunnels are generally run at low speeds. Eq. 4 shows that for a 1:100 model in a wind tunnel, the model velocity would be 100 times smaller than at full scale. In a water flow, the same Reynolds number can be achieved with a flow speed 1/10 of that in air, since the kinematic viscosity of water is approximately 1/10 that of air. The ability to use lower velocities will help scale buoyancy effects, discussed below.

Richardson number scaling

Buoyancy and stratification often play an important role in dispersion processes. The relative influence of buoyancy-induced and mechanically-induced velocity fluctuations (e.g., turbulent fluctuations resulting from the presence of mean shear) is expressed with the Richardson number. In air flows, the temperature gradients lead to strong density gradients that can lead to buoyantly driven flows. The gradient Richardson number is then given by:

$$\mathrm{Ri} = \frac{(g/\theta)(\partial\theta/\partial z)}{(\partial u/\partial z)^2} \tag{5}$$

where g is the gravitational constant, θ is the normalized temperature difference, $\partial u/\partial z$ is the velocity gradient, and $\partial\theta/\partial z$ is a temperature gradient. When Ri = 0, the flow is neutrally stable, when Ri > 0, stable stratification can occur, and when Ri < 0, convectively unstable flow can occur. In many flows, Ri < 0.25 indicates that there will be strong buoyancy-induced flows. The Richardson number can also be expressed in terms of the bulk flow properties:

$$\mathrm{Ri_B} = \frac{g(\Delta\rho/\rho)L}{(\Delta U)^2} \approx \frac{g(\Delta\theta/\theta)L}{(\Delta U)^2} \tag{6}$$

where ΔU and $\Delta\rho$ are the bulk velocity and density differences over the length scale L. The Richardson number can also be expressed in terms of the Froude number, which is the ratio of the gravitational and inertial forces:

$$\mathrm{Fr} = \frac{U^2}{gL} = \frac{\theta}{\mathrm{Ri}} = \frac{\Delta\rho}{\rho}\frac{1}{\mathrm{Ri_B}} \tag{7}$$

In model scale flows, the bulk Richardson number of the inflowing atmospheric boundary layer must be varied between $0 < \mathrm{Ri_B} < O(10)$ in order to replicate atmospheric near-surface stratification. This is achieved in wind tunnels through heating and cooling of the air, since the mean density of the air is nearly proportional to the mean temperature (in a nearly constant pressure flow). Relatively large temperature must be achieved with reported differences as large as 40 C (Robins et al., 2001). In water flows, the stratification is usually achieved through the use of brine and alcohol solutions. With $0.15 < U < 0.3$ m/s, and $0.01 < L < 0.1$ m, the required variation in the density is $0 < \Delta\rho/\rho < 20\%$. This is readily accomplished with brine/water/alcohol systems liquid (see, for example, Strang and Fernando, 2001)

When the dispersion of dense gases is considered, a Richardson number can also be defined based on the density difference between the ambient and dispersed gas.

Prandtl and Schmidt number scaling

The process of diffusion in fluids is related to the Prandtl and Schmidt numbers. The Prandtl number is given by:

$$\mathrm{Pr} = \frac{\rho C_p \nu}{k} \tag{8}$$

where C_p is the specific heat and k is the thermal conductivity. The Prandtl number presents the ratio of the viscous to thermal diffusivity. Similarly, the Schmidt number presents the ratio of viscous and molecular diffusion:

$$\mathrm{Sc} = \frac{\nu}{D} \tag{9}$$

where D is the molecular diffusivity.

Most of the dispersion flows under consideration are isothermal, so Prandtl number similarity need not be considered. When temperature gradients are used to create a finite Richardson number, the diffusion of heat throughout the domain must be managed, however.

The diffusion of passive contaminants requires consideration of the Schmidt number. The Schmidt number is a property of the fluid, not a flow parameter. Sc ~ O(1) for gases, while Sc ~ O(1000) for liquids. Thus, the *molecular* diffusion of contaminants is much lower in liquids compared to gases. However, the diffusion of contaminants in high Reynolds number flows is dominated by *turbulent mixing*. Breidenthal and Baker (1985) examined the scaling of turbulent mixing and entrainment and demonstrated that Schmidt number similarity is not necessary when the Reynolds number is sufficiently high to produce turbulent flow. As discussed above, this is also needed to achieve Reynolds similarity in the dispersive flows.

Rossby Number

The Rossby number is the relative influence of Coriolis forces on the flow. For large scale flows, the effect of the Coriolis force due to the Earth's rotation can be considerable. However, for smaller scale flows of 10 km or less, the influence of the Earth's rotation is felt through the imposed wind speed and direction on the surface layer. In that case, the Rossby number need not be considered.

Inlet Flow Boundary Conditions

Similarity between the model and full-scale atmospheric flows requires matching of the flow inlet boundary conditions. In wind tunnel testing, vortex generators and roughness elements are used to create an inlet flow with a prescribed mean flow profile with a given level and distribution of turbulent fluctuations. However, it is very difficult to replicate the variability of the atmospheric boundary layer with its changing wind direction and wide range of vortical scales. *This is a significant challenge for any testing method employing models.*

Atmospheric flows can be scaled with both air and water on the model scale. Table 4 summarizes how experiments in both air and water can be used to scale atmospheric dispersion. Here, it is assumed that the modeled domain (e.g., the test section cross section) has dimensions on the order of 1 m by 1 m, and flows of local scale or smaller are being modeled.

Scaling Issue	Range	Air Flow	Water Flow
Geometric Similarity	1:10 to 1:1000 scale factor	---	---
Reynolds Number	Re > $O(1000)$	1 to 3 m/s	0.1 to 0.3 m/s
Bulk Richardson Number	$0 < Ri < O(10)$	Temperature Gradients 10 to 100 C/m	Density Gradients $0 < \Delta\rho/\rho < 0.20$
Prandtl and Schmidt Number	Not scaled if Re > $O(1000)$	---	---
Rossby Number	Not Scaled	---	---
Inlet Boundary Conditions	1:10 to 1:1000 of the ABL flow.	Simulated Inlet Atmospheric Boundary Layer	Simulated Inlet Atmospheric Boundary Layer

Table 4: Parameters for air and water flow model similarity.

COMPARISON OF MODEL TESTING IN WATER AND AIR

At the present time, most dispersion model testing is conducted in low speed meteorological wind tunnels simulating neutral atmospheric boundary layers. This is largely due to the relative simplicity of wind tunnel testing compared to testing with water flows. Much of the testing that is performed involves determination of the *average* concentrations developed downstream of a *continuous* emission of contaminant. The data needed to evaluate Gaussian plume models are relatively modest and can be collected with a few point measurement devices. However, characterization of a transient dispersion event in a complex urban environment requires the collection of a much more varied and complete data set. Ideally, the model experiment would yield data with both *high spatial and temporal resolution*. Table 5 lists some common flow diagnostics used in wind tunnel flow testing.

Instrument	Quantity Measured	Spatial Resolution (m)	Temporal Resolution (s)
Pitot Tubes	**Single Point** Flow Velocity	0.01 to 0.001	> 1
Hot Wire Anemometers	**Single Point** Flow Velocity and Fluctuations	< 0.001	< 0.001
Laser Doppler Velocimeter	**Single Point** Flow Velocity and Fluctuations	< 0.001	< 0.001
Flame Ionization Detector	**Single Point** Tracer Concentration	0.001	> 1

Table 5: Diagnostics often used in wind tunnel dispersion studies.

These diagnostics are single point measurements, and note that the Laser Doppler Velocimeter is the only non-invasive flow diagnostic. *Average* velocity and concentration *fields* must be reconstructed by using multiple probes or by traversing the probe throughout the flow domain. This process is often cumbersome and time consuming. If stratification is achieved in the wind tunnel through the use of heated surface and temperature gradients, optical access can be reduced, making LDV measurements difficult. Strong temperature gradients also complicate the use of hot wire anemometers.

During the last ten years, researchers have developed flow diagnostics that can be used to measure *instantaneous* velocity, density, and concentration *fields*. Velocity fields can be measured using Particle Imaging Velocimetry (PIV), and density and concentration fields can be measured using Laser Induced Fluorescence (LIF) and Spectroscopy. Sheets of pulsed laser light are used to interrogate the flow field. Then, the recorded motion of many small Lagrangian flow tracers can be used to map out the velocity and vorticity fields**.** Figure 11 shows an example of combined PIV and PLIF taken of a large scale helium plume. This data was acquired as part of a Sandia program to provide validation data for fire and buoyant turbulence modeling (O'Hern et al., 2004). This high resolution, temporally resolved data is being used to validate models of turbulent fires. Laser induced fluorescence can be used to measure the presence of minute quantities of flow constituents. Both of these techniques can be used in airflows, *but they are much more readily implemented in water flows*. It is much easier to seed water flows with neutrally buoyant velocity seed particles and fluorescent dyes compared to airflows. In addition, the measurement of tracer mixing and dispersion can be performed with much more accuracy and sensitivity in liquids. Finally, stratification can be achieved in water flows while maintaining optical access.

Measurement of instantaneous velocity, density, and concentration fields will permit the evaluation of both the average flow quantities as well as their distribution in time. Moreover, fluctuations in the local concentration can be related to the corresponding unsteady velocity and vorticity fields. Development and validation of urban dispersions models requires such high fidelity data.

The use of water as a test fluid to simulate atmospheric and other air dispersion issues is not unprecedented. For example, Macdonald et al. (2000, 2002) used a water flume to study urban dispersion due to point releases in a regular array of cubes and the merging of buoyant plumes at 1:500 scale. O'Halloran et al. (2002) and Thatcher et al. (2004) have performed experiments on building interior room flows using scaled water experiments. Thatcher et al. (2004) provide an analysis of Reynolds number scaling and its effect on scaling of time and turbulence. However, in both of these cases the interest was in mechanically driven flows and thermal and stratification effects were neglected. Another difference between interior and exterior flows is the relative importance of molecular diffusion. As discussed above, in turbulent external flows turbulent mixing is much stronger than molecular diffusion. This will not always be the case in interior flows. McDonald et al. (2002) used a water flume to study at 500:1 scale the interaction of rising buoyant plumes.

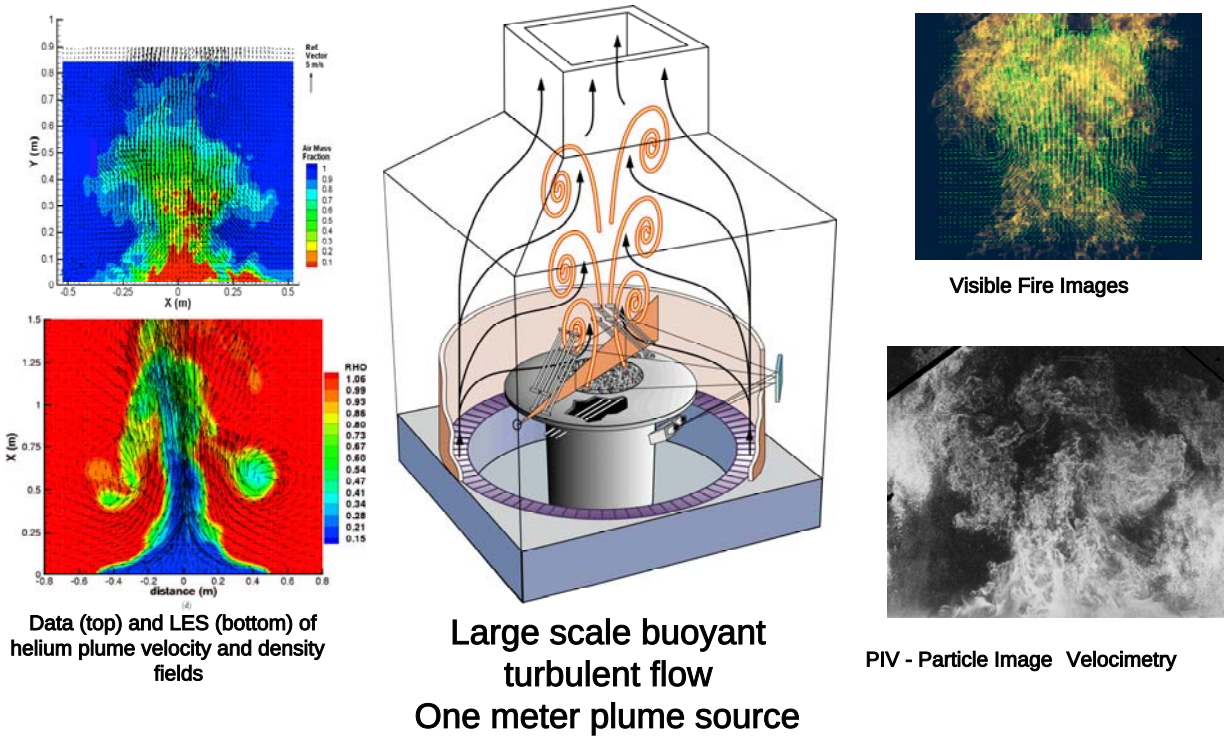

Figure 11: Example of PIV and PLIF images used to validate models of turbulent combustion (O'Hern et al., 2004).

Air is compressible (significant changes in density with pressure) while water is incompressible. However, water can a useful simulant for air (wind) for any reasonable wind situations; compressibility issues arise only at high Mach numbers, *e.g.*, when flow speeds reach, say, 10% of the sound speed 760 MPH at sea level (Liepmann and Roshko, 1957).

A WATER CHANNEL FOR THE STUDY OF URBAN DISPERSION

Because of the potential advantages of using water flows to model atmospheric dispersion, we have performed a conceptual design of a water flow test facility. Ideally, the test section would be on the order of 1 m by 1 m by 10 m, with a turbulence stimulation system upstream of the flow model. The maximum average flow velocity would be ~1 m/s. The test section would be designed to permit maximum optimal access for optical flow diagnostics. Stratification of the flow would be achieved through the use of multiple layers of fluid with varying density.

In continuing work in this LDRD project, we propose construction of a smaller-scale version of such a facility (**Figure 12**). This smaller facility would be used to validate the proposed tunnel design and demonstrate the use of modern optical diagnostics for dispersion flows. Of particular concern will be the creation of a stratified inlet boundary layer using a series of brine layers.

Diagnostics will include concentration measurement with a miniature fiber optic UV-VIS-NIR spectrometer or equivalent, laser-based techniques for velocity measurement (LDV and PIV), and noninvasive concentration (PLIF). The point concentration device will be mounted on a

traverse to allow plume source tracking using the computational algorithms being tested in this

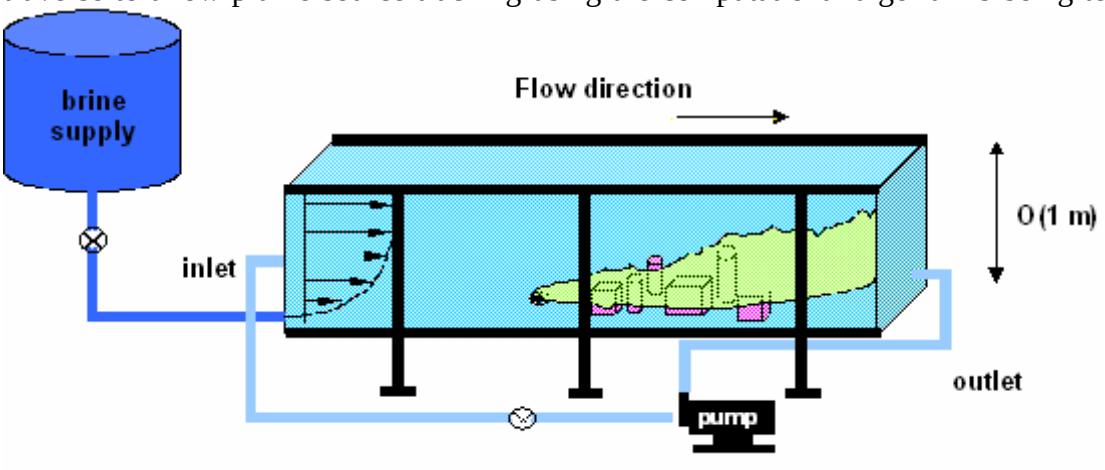

Figure 12: Schematic diagram of a demonstration dispersion water flow facility.

program. Concentration sampling taps could be located anywhere within the plume-affected region and could be multiplexed to a detector. Flow visualization will also be employed to provide global information on the plume behavior, building wake trapping effects, etc. The detailed design of the prototype flow facility is underway. This facility will have a smaller test section area and length. This smaller channel will be used to explore the following:

- The creation of the inlet stratified layers
- The development of the inlet mean and turbulent velocity profiles.
- The interaction of stratified layers with the developing boundary layer.
- The creation of a test section and flow models with the highest degree of optical access.
- The development of PIV and PLIF techniques for complex flows between obstacles.
- The development of PIV and PLIF techniques for the stratified flows.
- The possible recovery of brine downstream of the test section.

The successful implementation of the prototype facility would provide guidance for any subsequent implementation in a larger scale facility.

We will explore the use of optical index-matching fluids for the study of neutral dispersion flows. It is possible to construct the terrain and test models out of a solid material that has a matched optical index of the surrounding fluid, and light would pass through both the fluid and solids with minimal refraction (Budwig, 1994). Small-scale laboratory experiments have been performed with a variety of liquid-solid combinations. Researchers at INEEL operate a large-scale Matched Index of Refraction (MIR) flow facility (Knight et al., 2002; Zollinger, 2003). The facility uses constant temperature mineral oil as the flow medium in order to match the refractive index of quartz models. The temperature of the oil must be closely controlled. Researchers at Johns Hopkins have developed an MIR facility to study turbo-machinery (Uzol et al., 2002). Here, the liquid is a NaI and water solution, and the solid is acrylic. Both LDV and PIV have been used successfully to interrogate between blade rows with complex geometry.

MODELING NEEDS FOR DATA

As part of this effort, we contacted several researchers actively involved in the development and use of numerical dispersion models. Discussions were held with the following individuals:

- Dr. Richard Griffith, SNL
- Dr. Jay Boris, Naval Research Laboratory
- Dr. Michael Brown, LANL
- Dr. Gayle Sugiyama, LLNL
- Dr. Teresa Lustig, Department of Homeland Security
- Professor Darryl James, Texas Tech University

There was general agreement that good validation data is needed for the evaluation of all types of dispersion models. This is especially true for the case of transient releases in complex environments. Since large-scale outdoor testing is both challenging and expensive, the number of these tests will be limited. Consequently, there is likely to be a continuing need for model scale experimental data.

CONCLUSIONS

The scaling arguments provide justification that city-scale atmospheric dispersion phenomena can be successfully simulated using a laboratory-scale liquid flow facility. The use of a liquid flow facility would permit the application of modern full-field flow diagnostics such as Particle Image Velocimetry and Laser Induced Fluorescence toward the study of dispersion in complex environments. Liquid flows also allow for the simulation of stratified flows through the use of water, alcohol, and brine solutions.

The implementation of a liquid flow facility is more challenging than the creation of a wind tunnel of similar dimensions. However, a water flow facility has the potential to reveal the spatial and temporal evolution of continuous and transient gas emissions in extreme detail. With such data in hand, it will them be possible to critically evaluate the predictive capabilities of both simple and complex numerical dispersion models.

NOMENCLATURE

C_P	specific heat at constant pressure
D	molecular diffusivity
Fr	Froude Number
k	thermal conductivity
g	gravitational acceleration
L	characteristic length
L_{MO}	Monin-Obuhkov length scale
Pr	Prandtl Number
Re	Reynolds Number
Ri	Richardson Number
Ri_B	Bulk Richardson Number
Sc	Schmidt Number
u	local velocity magnitude
U	characteristic velocity magnitude
ΔU	change in velocity
z	spatial coordinate
z_o	roughness length scale

Greek Symbols

μ	absolute viscosity
ν	kinematic viscosity
ρ	density
$\Delta\rho$	change in density
θ	normalized temperature difference

Subscripts

p	prototype
m	model

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