Microscopic Aspects of Turbulent Transport –Atmospheric Dispersion of Pollutants – Part 2

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Abstract: A turbulent scalar transport model is proposed which is based on the analytical framework provided by spectral theory of turbulence and penetration theory. The new phenomenological model unifies diffusion and convection terms in a single transport equation, incorporating molecular properties of the diffusing scalar. In describing the turbulent dispersion of gases in atmospheric turbulent boundary layer, a concept of two turbulent time scales is introduced. The dispersive time scale for horizontal dispersion in the atmosphere is taken to be the reciprocal of geostrophic frequency, a well known parameter in earth science. The dissipative time scales for various stability classes are determined using Pasquill-Gifford experimental correlation. Proposed model predicts horizontal dispersion coefficient under various stability conditions within ± 20 % of Random Force theory. Model is extended for vertical dispersion using bulk Richardson number which seems to perform reasonably well.

Key-Words: Turbulent Diffusion, Mass Transfers, Atmospheric Dispersion, Convection,

1. INTRODUCTION

A general consensus has developed on the theory of molecular diffusion, in that molecular collisions and the consequential exchange of momentum and energy between molecules is the fundamental mechanism responsible for diffusion. Therefore, diffusion of a binary mixture of gases depends on their mutual collision cross section, an intrinsic property of the mixture[1]. Although various independent strategies can be adopted for estimating the rate of turbulent transport under specific flow conditions, there is no generally acceptable model for turbulence [2]. Three major theories, from which most of the analytical turbulent transport models are derived (i.e., statistical, similarity and the gradient transfer theories) emphasize flow characterization and properties of the bulk fluid and ignore any dependency on the microscopic characteristics of the mixture. It is well known that on a micro level the phenomenon of scalar transport is a molecular process. As Treylab [3] pointed out, molecular diffusion, is the ultimate process. Many attempts have been made to establish an analogy between Brownian motion and turbulent diffusion [4]. One such theory proposed by Gifford [5] has drawn considerable attention for modeling atmospheric dispersion. These models develop analogies with the conventional description of molecular diffusion which, for large time, simplifies to:

$$\sigma_M = \sqrt{2\, D_{AB}\, t} \tag{1}$$

where σ_M is the molecular dispersion coefficient, D_{AB} is the mutual molecular diffusivity of the species A & B, and t is the diffusion time. This paper proposes an alternative analytical approach for modeling turbulent transport of a passive scalar, which is very similar to Eq. (1) suggesting that molecular diffusion is in fact the limiting case of turbulent transport.

2. THEORY

In the present mathematical development, it is proposed that each state of turbulence can be represented by a characteristic energy spectrum, which describes all significant transport properties of the flow. This energy spectrum is associated with a set of characteristic time scales; therefore, it is argued that transport characteristics of a flow field can be represented by these time scales.

There is general agreement that the rate of molecular diffusion is limited by the available free energy (i.e. Gibb's free energy $\kappa\theta$). It is further argued that the excess energy required for accelerated turbulent dispersion arises from the dissipation of eddies as they cascade to smaller scales. Molecular collisions are responsible for the transfer of energy and momentum from the bulk fluid molecules to the mixing scalar, which results in their transport and diffusion in the bulk fluid. Therefore, it is necessary to incorporate the molecular characteristics of the mixture in a rigorous mathematical model for turbulent transport. This approach is a significant philosophical improvement to most current turbulent transport models, which focus mainly on the flow characteristics and ignore any dependency on intermolecular properties of the mixture.

The proposed model for turbulent transport is based on the following assumptions:

A) In a fluid medium, intermolecular collision is the fundamental mechanism of energy and momentum transfer between molecules; therefore, convective or turbulent transport phenomenon is also influenced by intermolecular characteristics of the mixture;

B) The driving force for turbulent dispersion is related to the rate of energy dissipation in the flow field;

C) Turbulence is best represented by energy spectrum function that characterizes the distribution of energy amongst eddies of various sizes;

D) Gravity/buoyancy is the only additional factor that influences vertical dispersion.

3. Time Scales

Although turbulent phenomena are governed by a wide range of time and length scales, most of the conventional models for turbulent transport utilize only a single time (or length) scale. In this paper, turbulent diffusion is modeled using two independent time scales; the *Dissipative Time Scale* and the *Integral or Dispersive Time Scale*. Two time scale approach is similar to the *Multiscales Methods* [6], however, available literature does not associated any physical significance to these various scales.

The physical existence of two independent time scales can be established by using Gifford's [5] expression for the rate of energy dissipation, $\varepsilon \sim \overline{v^2}/T_L$ and eddy diffusivity, $K = \overline{v^2}\, T_L$, where ε is the rate of energy dissipation per unit mass, $\overline{v^2}$ is the mean square velocity, and T_L is the *Lagrangian integral time scale*. Thus, $K = \varepsilon\, T_L^2$. For homogeneous stationary turbulence, the average energy dissipation rate per unit mass is estimated by:

$$\varepsilon = 2\,\nu \int_0^\infty k^2 E(k)\, dk \tag{2}$$

where $E(k)$ is the energy spectrum defined by the Fourier transform of the correlation function [7, 8]. $E(k)$ can be obtained by using the asymptotic form of the correlation function used by Gifford [5], and others [9] :

$$R(\tau) = e^{\tau/T} \tag{3}$$

The Fourier Transform of Eq.(3) gives the following expression for one dimensional energy spectrum;

$$E(k) = \frac{4\,T}{1+\left(2\,k\,\pi\,T\right)^2}$$

This energy spectrum can then be used in Eq. (2) to obtain ε. Substituting ε in the expression for eddy diffusivity yields:

$$K = \varepsilon\, T_L^2 = \frac{\nu}{2\,\pi^2\,T^2} T_L^2 \tag{4}$$

Since values reported for eddy diffusivity (K) are orders of magnitude larger than the kinematic viscosity (ν) one must conclude that there are at least two independent time scales involved in the phenomenon of turbulent transport. The time scale, T, in the denominator of Eq.(4) is related to the rate of energy dissipation and is much smaller than T_L, which is associated with the phenomenon of eddy dispersion. The use of two time scales to describe turbulent diffusion is reasonable because the average scale of eddies being destroyed and dissipating their energy is much smaller than the corresponding scales of eddies responsible for large scale dispersion. Two time scales assumption can be readily tested by comparing the magnitude of various quantities in Eq.(4) for atmospheric diffusion, $K \sim 10^5$ m^2 sec^{-1}, $\nu \sim 10^{-6}$ m^2 sec^{-1} and $\pi^2 \sim 10^1$. Therefore, $\dfrac{T_L}{T_K}$ must be on the order of 10^6, which agrees well with reported [10] ratio of the two corresponding scales. Based on this comparison, it is believed that in *Similarity approach*, where eddy diffusivity is related to fluid viscosity by using a scaling factor, the scaling factor may possibly be the squared ratio of the two time scales.

4. Mathematical Model

Turbulent gas diffusion can be viewed as an interfacial phenomenon, where eddies from the bulk fluid penetrate the plume for a finite duration of time. During this time, a mass exchange takes place between the plume and the eddy. The proposed model assumes that the nature of this mass transfer is solely molecular. Afterwards, these eddies move away from the interface into the bulk fluid where smaller eddies penetrate them and the process is repeated. A cascade of eddy penetrations, molecular diffusions, and transport result in turbulent diffusion. It follows from this description of turbulent transport that the turbulent dispersion coefficient can be obtained by multiplying the expression for the turbulent scalar (mass) transfer coefficient with a characteristic time scale. Various theories for interfacial mass transfer were carefully examined to establish an expression for the mass transfer coefficient under turbulence. The common two film theory [11] was found to be inappropriate for this application because of the unrealistic concept of a stagnant film at fluid interface and the lack of film stability as expected under turbulence.

Higbie [12] recommended a *Penetration Theory* for estimating mass transfer at a liquid-gas interface. Using an appropriate choice of model parameters, Higbie's approach can be applied to estimate interfacial mass transfer for any two fluids. Penetration theory assumes that the fluid surface consists of small elements (i.e. eddies) that contact the other fluid at the interface for a given duration of time before being swept back into the bulk fluid and remixed. Each out-going fluid element is then replaced by another similar fresh element from the bulk fluid. A detailed discussion of the applicability of penetration theory is given by King [13]. Based on this discussion it is concluded that under turbulent flow condition penetration theory is applicable for modeling atmospheric mixing. Penetration theory leads to the following expression for the transient mass transfer coefficient:

$$K_T = \sqrt{\frac{D_{AB}}{\pi\, t}} \tag{5}$$

This unsteady-state model provides a reasonable approximation for mass transfer under turbulent conditions. The duration of eddy penetrations/exposures are typically small and an average mass transfer coefficient over the entire duration of exposure (i.e., T_k) is obtained by time integration of Eq.(5). The final expression is:

$$K_T = \frac{1}{T_k}\int_0^{T_k}\sqrt{\frac{D_{AB}}{\pi\, t}}\,dt = 2\sqrt{\frac{D_{AB}}{\pi\, T_k}} \qquad (6)$$

This paper assumes that the turbulent mass transfer coefficient for atmospheric diffusion can be expressed by penetration theory. Consistent with assumption A, penetration theory relates the turbulent mass transfer coefficient with intermolecular characteristics of the mixture, i.e., the mutual diffusivity, which in turn depends on the molecular collision cross section. It is postulated that a further correlation can be established by multiplying the mass transfer coefficient with an appropriate time scale to obtain the turbulent dispersion coefficient, that is:

$$\sigma_y = 2\sqrt{\frac{D_{AB}}{\pi\, T_k}}\; T_L \qquad (7)$$

where T_L is the *Lagrangian integral time scale,* a scaling factor which depends primarily on the flow geometry.

Prediction of the dispersion coefficient (Eq. 7) requires determination of the two time scales suitable for the specific geometry and flow conditions. Eddy exposure time (i.e., T_k) is related to eddies in the bulk fluid that penetrate the plume at the interface where some of the plume mass will diffuse into the eddy and be carried back into the bulk fluid. It is conventional to use Kolmogorov's [14] time scale for eddy exposure time scale [15, 16, 17] which is defined as:

$$T_k = \sqrt{\frac{\nu}{\varepsilon}} \qquad (8)$$

However, Yakhot [18] concluded that there exists an entire spectrum of the dissipative time scales and the Kolmogorov's time scale limit may not be physical. Usman [19] also suggested an entire spectrum of dissipative time scales, the average of which describe the mean transport rate for specific fluid and flow geometry. The average dissipative time scale is related to the fluid kinematic viscosity ($\nu = \frac{\mu}{\rho}$) and the rate of energy dissipation (ε) from all the dissipating scales. Consistent with our assumption B, we propose to use the average dissipative time scale $\overline{T}_k$ for the average eddy exposure time, which makes the diffusion rate a function of the energy dissipation rate. The mixing or dispersive time scale in Eq.(7), T_L, is associated with the phenomenon of dispersion and is often approximated by Lagrangian integral time scale:

$$T_L = \int_0^{\infty} R(\tau)\; d\tau \qquad (9)$$

For a point source, dispersion and the corresponding time and length scales are dynamic functions of the travel time. For the specific case of zero initial velocity, both Papoulis[20] and Gifford[5] proposed the following autocorrelation function:

$$R(\tau,t) = e^{\frac{-\tau}{T_L}}\,(1 - e^{\frac{-2t}{T_L}}) \qquad (10)$$

This makes velocity autocorrelation a function of travel time, which appears to contradict the assumption of stationary turbulence. The literature, however, does not adequately stress that this velocity autocorrelation function is for a parcel of "pollutant" or an external scalar introduced into the bulk flow at time t = 0. The term outside the parentheses of Eq.(10) represents the correlation function for the bulk fluid in turbulent motion. For the case of zero initial velocity, all pollutant particles are in random (or Brownian) motion with a Maxwellian velocity distribution having a zero mean velocity. Initially, the velocity correlation among the pollutant particles is also zero. As time progresses, the turbulent flow field starts to affect the pollutant by transporting it along with the bulk fluid. The velocity distribution of pollutant particles will also change and exhibit a positive mean velocity in the direction of bulk flow. As the term $(1 - e^{\frac{-2\,t}{T_L}})$ approaches unity, both the mean velocity and the autocorrelation function approach asymptotic values equal to that of the bulk fluid.

Saffman [21] arrived at similar results based on his argument that molecules of a diffusing "substance" behave differently than the fluid particles. His intuitive expression (in his own words) resembles Eq.(10). He also concluded that the interaction between molecular diffusion and turbulence can reduce dispersion. Saffman is the first one to recognize the interaction of molecular and turbulent diffusion from a statistical view point. His analysis, and almost all the other existing literature, is based on the assumption that turbulent and molecular diffusion are "independent and additive" processes. Usman et. al. [22] have questioned the assumption of mutual independence of turbulent and molecular diffusion by suggesting that turbulent and molecular processes are manifestation of the same microscopic phenomenon (i.e. molecular scattering).

Incorporating the time-dependent form of velocity autocorrelation function into Eq.(9), the expression for the Lagrangian time scale for the y direction (i.e. horizontal direction perpendicular to mean velocity) can be written as:

$$\begin{aligned} T_L^y &= \int_0^{\infty} e^{\frac{\tau}{T}}\,(1 \quad e^{\frac{2\,t}{T_L}})\,d\tau \\ \therefore T_L^y &= (1 \quad e^{\frac{2\,t}{T_L}})\; T_{L\infty}^y \end{aligned} \qquad (11)$$

where $T_{L\infty}^y$ is the asymptotic value of the Lagrange integral time scale in y direction. It should be noted that the vertical asymptotic integral time scale ($T^{z}_{L\infty}$) may be quite different from $T^{y}_{L\infty}$ as the scale of vertical waves are limited by the depth and stratification of the planetary atmosphere. Incorporating these time scales in the model, the final expression for the dispersion coefficient becomes:

$$\sigma_y = 2\sqrt{\frac{D_{AB}}{\pi\,\overline{T}_k}}\ (1-e^{\frac{-2t}{T^{y}_{L\infty}}})\ T^{y}_{L\infty} \qquad (12)$$

The average dissipative time scale (i.e., $\overline{T}_k$) is a critical parameter defining the state of turbulence. As Usman [19] and Yakhot [18] recognized the existence of an entire spectrum of dissipative scales, therefore, an averaging is necessary to estimate the transport characteristics of the flow. The average dissipative time scale depends on the rate of energy dissipation, which, in turn, is a function of the kinematic viscosity of the fluid and the energy spectrum. The energy spectrum, $E(k)$, fully expresses the transport characteristics of the flow. This is consistent with our assumption C.

5. Model Extension for Vertical Dispersion

For vertical atmospheric dispersion, in addition to mechanical turbulence caused by surface roughness, thermal turbulence also contributes to the process of dispersion, and may at times become the dominant contributor [23]. Fluctuations due to mechanical turbulence tend to be relatively small and quite regular [23]. However, large mechanical eddies are also possible in rough terrain. Thermal eddies are both larger and more variable in size than the most mechanical eddies [23].

The presence of thermal waves or eddies further enhances vertical dispersion. This augmentation is weak when the atmospheric lapse rate approaches the *adiabatic lapse rate*. The adiabatic lapse rate for dry air is reported to be approximately -0.98^{o} per 100 meters [23, 24]. Lapse rates greater than adiabatic (unstable condition) induce buoyancy which forces a displaced parcel of air to continue its motion. On the other hand, during stable conditions, the lapse rate is smaller than adiabatic lapse rate, and a displaced parcel of air is forced to return to its original position.

Thus, an unstable condition is expected to enhance diffusion, a stable condition tends to suppress mechanical diffusion, and a neutral condition has no contribution from thermal turbulence and dispersion is only caused by mechanical turbulence. It is conventional practice to characterize atmospheric stability by use of the Richardson Number [25], R_i, which represents the ratio of the relative importance of buoyancy or convective turbulence to mechanical turbulence [26]. Alternatively, the bulk Richardson Number or Monin-Obukhov [27] length can be used to characterize atmospheric stability.

Under extremely unstable conditions the enhancement of vertical diffusion is more pronounced, as mechanically displaced parcel of pollutant will continue its motion as a result of buoyancy. This can be regarded as an elongated eddy, oval in shape with the major axis in z-direction. In other words, presence of thermal eddies tends to increase the average dispersive time scale in the vertical direction. The effective or pseudo time scale for vertical dispersion is a function of the actual time scale and a stability parameter such as Monin-Obukhov length [27] or Richardson number [25]. Furthermore, for unstable conditions, the buoyancy effect is compounded with time such that thermal turbulent displacements keep multiplying with travel time. Therefore, a pseudo dispersive time scale becomes a dynamic function of travel time. For unstable conditions, it is therefore proposed that:

$$T^{z}{}_{Eff} = e^{\frac{\left|Ri_{Avg}\right|\,t}{T_L}}\ T^{z}_{L\infty} \qquad (18)$$

where $T^{z}{}_{Eff}$ is the effective dispersive time scale and Ri_{Avg} is the average bulk Richardson number. If buoyancy is the only additional factor involved in the vertical dispersion (consistent with our assumption D), then by using this effective dissipative time scale the final expression for the vertical dispersion coefficient under unstable conditions becomes:

$$\sigma_z{}^{Unstable} = 2\sqrt{\frac{D_{AB}}{\pi\,\overline{T}_k}}\ e^{\frac{\left|Ri_{Avg}\right|\,t}{T^{z}_{L\infty}}}\ (1\quad e^{\frac{2\,t}{T^{z}_{L\infty}}})\ T^{z}_{L\infty} \qquad (19)$$

For neutral conditions the Richardson number approaches zero which eliminates the extra exponential term and the equation reduces to the expression for the horizontal dispersion coefficient. Stable conditions tend to suppress mechanical eddies. This suppression would slow down the vertical eddies and reduce the magnitude of the dispersive time scale. This situation can be visualized as an oval shaped eddy with minor axis in z-direction. As a result of this shorten eddy, the dispersive time scales time scale for vertical direction would reduce. However, the compounding effect of dispersion enhancement seen in unstable condition would not exist. Therefore, dispersion under stable conditions can be modeled using the expression for horizontal dispersion and an appropriately adjusted time scale to account for the effect of thermal suppression. The equation vertical dispersion under neutral and stable conditions therefore becomes:

$$\sigma_z = 2\sqrt{\frac{D_{AB}}{\pi\,\overline{T}_k}}\ (1\quad e^{\frac{2\,t}{T^{z}_{L\infty}}})\ T^{z}_{L\infty} \qquad (20)$$

6. Model Comparison with Atmospheric Data

Vogt [28] compiled a list of generally accepted atmospheric dispersion experiments. Most of the dispersion observations were made for a limited source receptor distance, while predictions for dispersion are required for distances that are orders of magnitude greater than those observed. Because of limitations inherent in the measurements, results of atmospheric dispersion experiments are often reported in form of an empirical correlation. There are at least five such systems of empirical correlation [24] in use for estimating dispersion coefficients. Experimental data is usually divided into six discrete categories based on the meteorological conditions as proposed by Pasquill [29]. Correlations proposed by Gifford [30], commonly known as Pasquill-Gifford curves (P-G curves) are most widely used world wide. P-G curves are graphical representation of dispersion coefficient under various atmospheric stability conditions as a function of downwind distance. While the model described in this paper relates the dispersion coefficients with travel time. Distance to time dependency conversion was made using the average wind velocities [19].

It has been suggested [31, 32, 33] that the integral time scale for atmospheric dispersion, ($T^{y}_{L\infty}$), is of the same order of magnitude as the reciprocal of the geostrophic frequency (i.e., the frequency of earth rotation). Their suggestion is logical, in that the time scale of earth rotation is the largest scale conceivable for atmospheric flow. Panofsky [8] has also expressed similar view by relating the depth of the Planetary Boundary Layer (PBL) with Coriolis parameter, f . Thus, the dispersive time scale for the horizontal direction adopted in the present model is approximately 24 hours ~ 10^4 seconds. A value for the average dissipative time scale,$\overline{T}_k$, for each stability class was determined by performing a linear regression of the proposed model predicted dispersion coefficients against the P-G curves, using the Marquardt-Levenberg algorithm. Based on this regression, best values for dissipative time scales were determined that would minimize the over error between the model prediction the experimental results. Best values for dispersive and dissipative time scales for horizontal dispersion coefficient under each stability class were obtained as shown in Table 1.

The assumption of isentropic turbulence at small scales requires that the vertical dissipative time scales under each stability class must be the same as their horizontal counterparts. Therefore, horizontal dissipative time scales determined by regression were also used for the respective vertical dissipative time scales under various stability classes. However, for vertical dispersion, it is unreasonable to use the reciprocal of geostrophic frequency as dispersive scales because the vertical dimension available for dispersion/mixing is quite different than the horizontal space. Furthermore, under different stability conditions, the vertical length and time scales change depending on thermal stratification. For that reason, use of a single value for the vertical dispersive time scale ($T^{z}_{L\infty}$) under all stability condition was also considered to be inappropriate. Therefore, for vertical dispersion, the dispersive time scales ($T^{z}_{L\infty}$) under each stability condition were determined by regression. Likewise, an estimated value for the average bulk Richardson number was also determined for unstable conditions (i.e. Stability Class A & B). These parameter values for vertical dispersion are listed in Table 1. These values were used to predict dispersion coefficients under various stability classes. Predictions of dispersion coefficients generated by the proposed model with those from other well known correlations (including the P-G curves) are shown in Figures 1 and 2.

7. Discussion of Results and Parameter Effect:

Figures 1 illustrates that model predictions for the horizontal dispersion coefficients are within ± 20% of Gifford's Random Force Theory [5] over nearly the entire range of interest for all six atmospheric stability classes. Error bars of ± 20% are added to the predicted results. It is obvious that the model performs reasonably well for all stability classes. However, the agreement is best for unstable atmospheric conditions, i.e., stability class A. As the atmosphere becomes stable (classes E and F), the model begins to deviate from the empirical results. As seen in the figure, inter-comparison of the various empirical correlations also starts to exhibit discrepancies for highly stable conditions.

Somewhat of a poor model performance for highly stable condition is quite understandable, because the model described in this paper is based on penetration theory for computing mass transfer coefficients which is suitable for high turbulent conditions [12, 34]. It is believed that two-film theory may be more appropriate for stable conditions.

Figure 2 illustrates model predictions for vertical dispersion coefficients with error bars of ± 20% for all six atmospheric stability classes. Model extension is based on the assumption that atmospheric turbulence is isentropic at small scales, therefore the dissipative time scale for vertical direction under a specific stability condition is identical to its horizontal counter part. And gravity/buoyancy is the only additional factor influencing vertical dispersion, which is modeled by using an effective bulk Richardson number.

The dispersive time scales for vertical dispersion are limited by the state of thermal stratification which depends on the stability conditions. Therefore, dispersive time scale for each stability condition was determined by regression of the model expression against the P-G curves. With this phenomenological modification, the extended vertical dispersion model seems to perform quite well.

Since the literature does not explicitly account for two independent time scales, it is difficult to compare the numerical values of the dissipative time scales used in the proposed model, however, our estimate for dissipative time scale in the range of 10^{-2} to 10^{-4} seconds, agrees with Nieuwstadt [10] and Panofsky [8] suggestion that the dissipative length scales in atmospheric flow is of the order of millimeters, and the corresponding time scales in the range of milliseconds. Recently Hall et. al [35] experimentally estimated the rate of atmospheric energy dissipation to be in the range of 10 – 100 mW/kg ,which leads to an estimated dissipative time scale of approximately 10^{-4} seconds. This estimate is in the same order of magnitude as that predicted by model regression against the empirical correlation.

It is also interesting to notice the trend in the dissipative time scale, which starts with a small value for the most unstable condition (resulting in a maximum energy dissipation rate) and increases as the flow approaches the most stable condition for which energy dissipation is minimum. Use of a single value for both horizontal and vertical dissipative time scales also supports the assumption of isentropic turbulence in atmospheric flow at small scales which also indirectly implies that the proposed model is a reasonable representation of atmospheric mixing phenomenon. Moreover, the values for the average bulk Richardson number used in this study are close to the values reported by Schreurs and Mewis [36].

For dispersive time scales, literature [37] reported a wide variation. For horizontal dispersion, the model uses a fixed value of 10^4 seconds for dispersive time scale as suggested by Gifford and co-workers [31, 32, 33]. This simple approach seems to perform very well. However, for vertical dispersion additional complexity is introduced due to thermal stratification. Recognizing the effect of thermal stratification in limiting the vertical length and time scales, a stability dependent dispersive time scale is determined for each stability class. In general, vertical dispersive time scales are an order of magnitude smaller than their horizontal counter part. This observation is supported by Draxler [26]. Moreover, there is a sharp decrease in the vertical dispersive time scales from neutral (stability C) to stable condition (stability class D) which is reported to be due to thermal suppression of turbulence in the atmosphere.

A significant feature of the present model is that it contains molecular diffusivity in the expression for the turbulent dispersion coefficient, which suggests that even turbulent transport is dependent on the molecular characteristics of the mixture. In view of the general agreement [3] that both molecular diffusion and turbulent mixing are manifestation of the same microscopic phenomenon i.e., molecular collision and scattering, the present development assumes that molecular and turbulent diffusion are closely related phenomena. In fact, it can be shown that molecular diffusion is the limiting case of turbulent transport. Starting with penetration theory's mass transfer coefficient without time averaging;

$$\sigma_y = \sqrt{\frac{D_{AB}}{\pi t}}(1 \quad e^{\frac{2t}{T^y_{L\infty}}})\, T^y_{L\infty}$$

Taylor's expansion approximation for short observation time would result;

$$\sigma_y = \sqrt{\frac{D_{AB}}{\pi t}(1 \quad (1 \quad \frac{2t}{T^y_{L\infty}} + ...))\, T^y_{L\infty}}$$

$$= \sqrt{\frac{4t^2 D_{AB}}{\pi t}} = Const. \sqrt{2 t D_{AB}}$$

The final result has an outstanding resemblance with equation (1), suggesting that for very small observation times, the observed dispersion is same as the molecular diffusion. This feature of the proposed model, obviously need further investigation.

8. Summary and Conclusions

A new model for predicting transport of passive scalar has been developed which includes molecular diffusivity in the expression for the turbulent transport, establishing a relationship between molecular diffusion and turbulent transport. The new model depends on only two coefficients, i.e., the dissipative time scale and dispersive time scale. Dispersive time scale is associated with the largest conceivable wave (or eddy) in the flow and hence is determined primarily by flow geometry. On the other hand, the dissipative time scales is related to the rate of energy dissipation and hence depends on the energy supply and the ability of eddies to cascade to smaller scales. Use of these two independent times scales and their physical interpretation had reduces the inherent empiricism that exists in most of the current turbulent transport models. For horizontal dispersion, the dispersive time scale is associated with the size of the largest possible eddy, the geostrophic frequency, which dependent on flow geometry. Therefore, the model actually depends only on one empirical parameter which is associated with the rate of energy dissipation in the flow field.

This model has a wide application in numerous areas of science and engineering and can readily be extended to heat transfer by using the thermal conductivity of the gas in place of diffusivity. However, the two time scales will have to be determined to adequately represent the flow geometry and the state of turbulence.

The proposed model when applied to atmospheric dispersion provides a plausible explanation for the observed slower dispersion of heavy gases [38] and suggests that the smaller molecular diffusivity of heavy gases may be responsible for their slower turbulent dispersion rates.

Atmospheric horizontal dispersion coefficients were predicted for all six Pasquill Stability using the appropriate choice of model parameters. With slight modification to account for the effect of buoyancy and/or gravity, the new model predicts vertical and horizontal dispersion coefficients that are in good agreement with empirical correlations.

Acknowledgement: The authors would like to thank Dr. Joel Weisman, Prof. James Anno (Late), and Prof. John Christenson for their encouragement, advice and review of the manuscript.

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Table 1.
Model Parameters for Horizontal and Vertical Dispersion

Pasquill Stability Class	Wind Velocity v(m sec^{-1})	Horizontal		Vertical		
		$\overline{T}_k^Y$	$T_{L\infty}^y$	$\overline{T}_k^Z$	$T_{L\infty}^z$	Ri_{Avg}
A	2.8	3.16 10^{-4}	1.00 10^{4}	3.16 10^{-4}	5.41 10^{3}	11.6
B	3.4	3.43 10^{-4}	- do -	3.43 10^{-4}	2.37 10^{3}	1.0
C	4.7	5.95 10^{-4}	- do -	5.95 10^{-4}	4.11 10^{3}	N/A
D	5.5	7.20 10^{-4}	- do -	7.20 10^{-4}	7.16 10^{2}	N/A
E	3.7	3.41 10^{-3}	- do -	3.41 10^{-3}	9.01 10^{2}	N/A
F	2.2	1.04 10^{-2}	- do -	1.04 10^{-2}	8.72 10^{2}	N/A

Nomenclature

Symbol	Description	Units	Symbol	Description	Units
σ_M	Molecular Dispersion Coefficient	L	$R(\tau)$	Autocorrelation function	
σ_y	Dispersion coefficient (i.e. $\sqrt{\overline{Y}^2}$)	L	t	Time (diffusion time or eddy exposure time for penetration theory)	T
σ_z	Dispersion coefficient (i.e. $\sqrt{\overline{Z}^2}$)	L	$T^z{}_{Eff}$	Effective dispersive time scale in vertical direction	
κ	Boltzmann's Constant		T_K	Dissipative time scale and eddy penetration exposure Time	
θ	Temperature	°C or K	T_L	Lagrangian integral time scale	
ε	Rate of energy dissipation per unit mass	L^2 T^{-3}	v	Velocity	
ν	Kinematic Viscosity	L^2 T^{-1}			
τ	Lag time for correlation coefficient	T			
D_{AB}	Mutual diffusion coefficient of gases A & B	L^2 T^{-1}			
$E(k)$	Energy spectrum in frequency domain				
k	Frequency	T^{-1}			
K	Eddy diffusivity	L^2 T^{-1}			
Ri	Richardson Number	-			
Ri_{Avg}	average bulk Richardson number				
Ri_{Bulk}	Bulk Richardson Number				

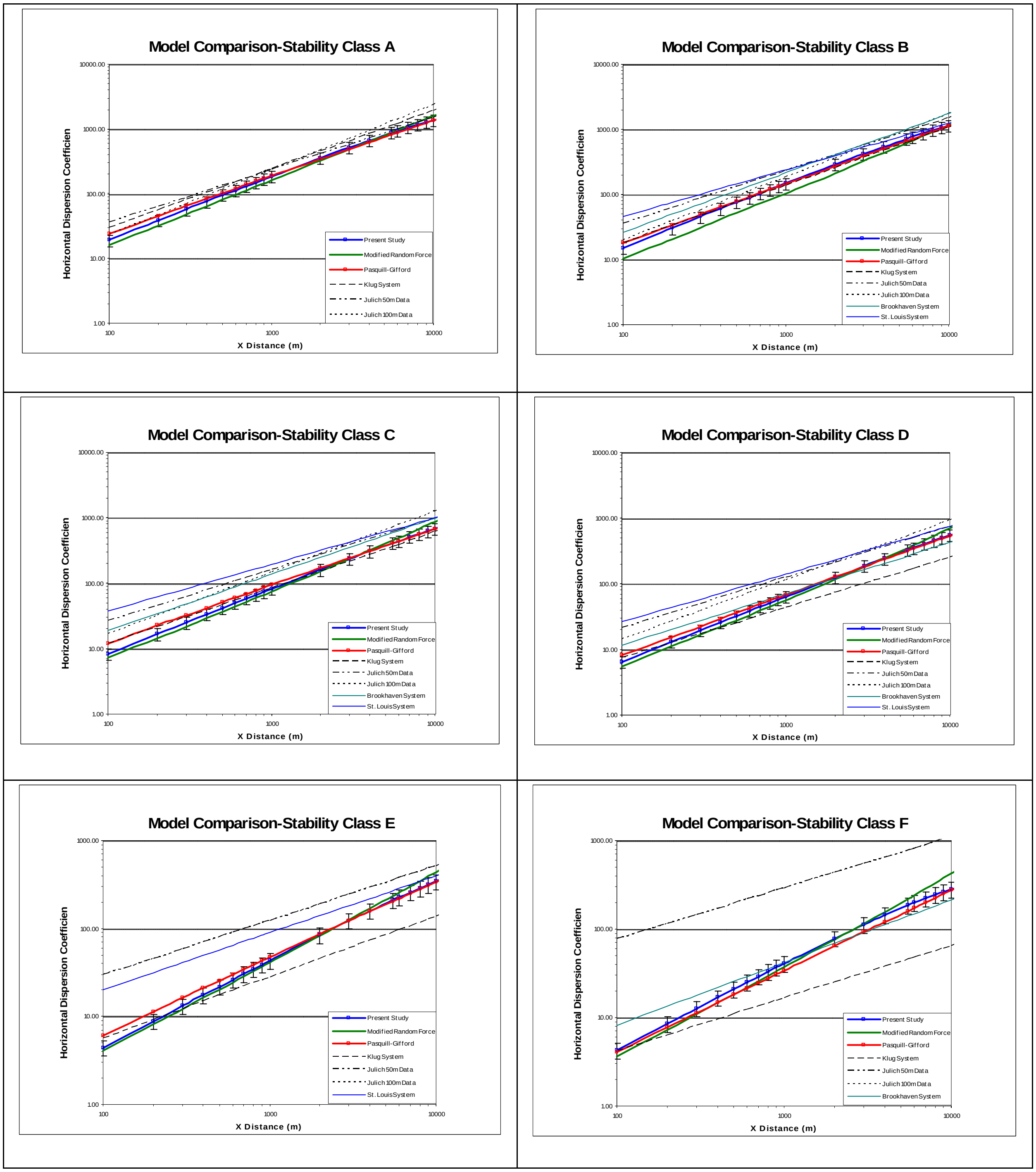

FIGURE 1
Comparison of Horizontal Dispersion Prediction

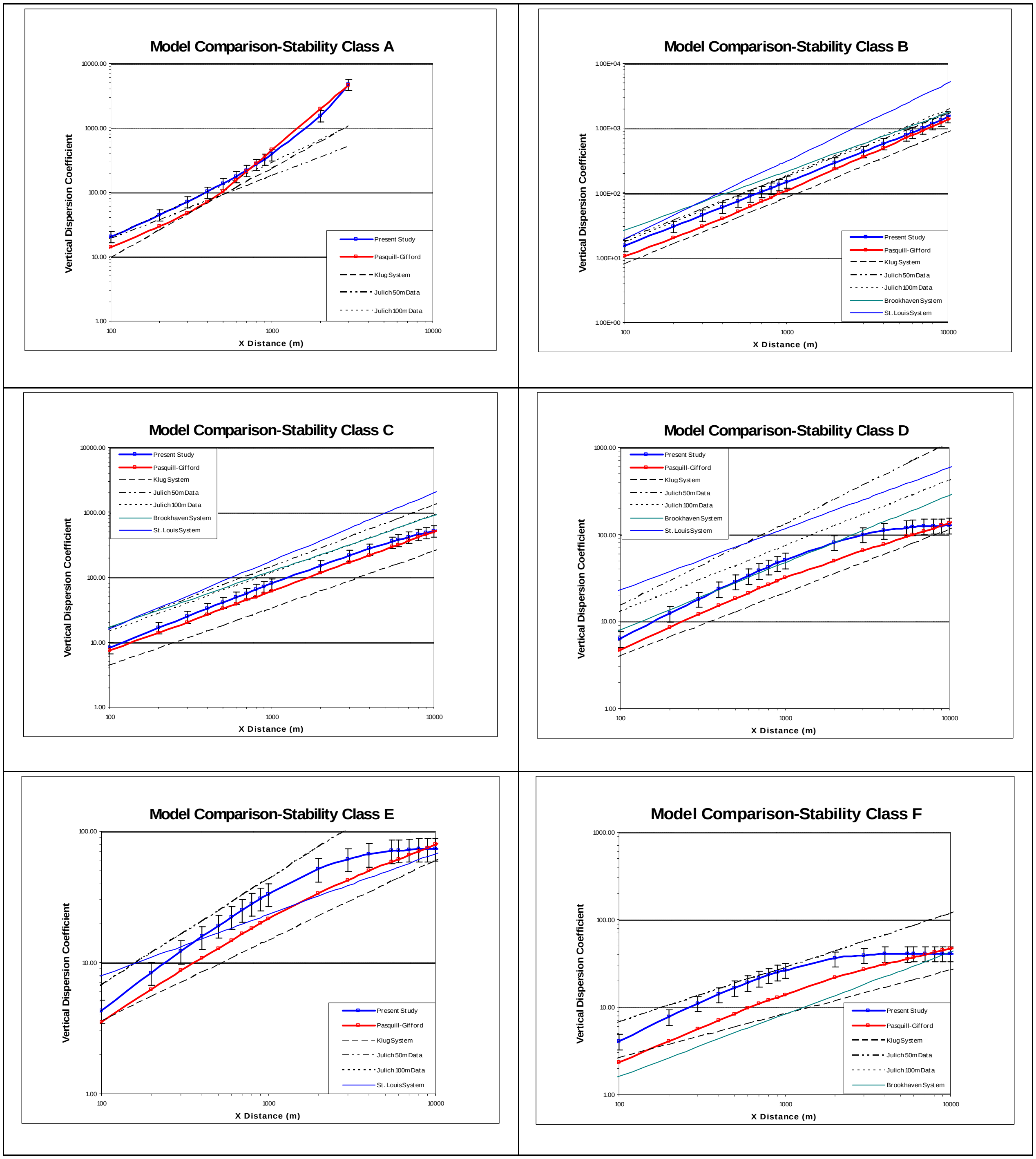

FIGURE 2

Comparison of Vertical Dispersion Prediction