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*Article*

# Generalized 3D Model of Crosswind Concentrations and Deposition in the Atmospheric Boundary Layer

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**Abstract:** In this paper, we introduce a comprehensive solution aimed at enhancing the understanding of three-dimensional atmospheric pollutant dispersion. This innovative solution develops a generalized model that extends previous research and is applicable to all parameterization schemes of the equation, including wind speed profiles and turbulent diffusion coefficients, while incorporating the dry deposition criterion. Our methodology involves subdividing the atmospheric boundary layer into distinct sublayers, which facilitates a detailed examination of pollutant dispersion dynamics. Extensive validation with data from the Hanford experiment has demonstrated the accuracy of this solution in simulating pollutant concentrations. The results exhibit a strong correlation between projected and observed concentrations, underscoring the statistical reliability of our approach. This validation situates the statistical indices of our solution within an acceptable range, confirming its accuracy in predicting atmospheric pollutant dispersion. These findings thus establish our solution as a valid and effective method for studying complex environmental phenomena.

**Keywords:** atmospheric parametrizations; atmospheric boundary layer; three-dimensional dispersion; turbulent dispersion; dry deposition; generalized analytical model; closed-form solution

## 1. Introduction

Understanding the dispersion, transport, and fate of atmospheric pollutants necessitates a thorough analysis of deposition processes. These mechanisms are essential in determining plume behavior and concentration patterns within the atmospheric boundary layer (ABL) [29]. However, Gaussian plume model estimates often fall short due to particle settling, deposition, or vertical gradients in diffusivity and wind speed [27]. The Earth's surface acts as the primary reservoir for trace gases and particles, which transfer through wet and dry deposition pathways. Wet deposition is driven by precipitation, whereas dry deposition involves the adhesion or chemical reaction of trace gases and particles on surfaces like vegetation, soil, water bodies, and structures. Factors such as atmospheric turbulence intensity, the properties of gases and particles, and surface characteristics influence the efficiency of dry deposition [24]. In the absence of turbulence, even surfaces with high adsorptive capacity are ineffective in removing suspended materials, as the process is limited by molecular diffusion. Gravitational settling also plays a role in the dry deposition of particles, further complicating these dynamics [10]. The role of deposition processes in the dispersion of passive contaminants within the ABL is conventionally modeled using the advection-diffusion equation, as dictated by gradient transport theory, with deposition fluxes incorporated as boundary conditions at the surface [9]. To address this, a modified Gaussian model was formulated, initially presuming constant wind speed and homogeneous eddy diffusivity [13]. For enhanced applicability, eddy diffusivities were subsequently adjusted based on dispersion parameters relative to the downwind distance, and wind speed was modeled using a power-law relationship with vertical height [17]. However, this method introduces mathematical inconsistencies due to the employment of unrealistic parameterizations [26].

In this paper, we present an innovative approach aimed at improving the understanding of pollutant behavior in the atmospheric boundary layer (ABL). Our research introduces a generalized, one-of-a-kind model capable of adapting to all existing parameterization schemes. This model holistically integrates various wind speed profiles, turbulent diffusion coefficients, and dry deposition

criteria, thereby offering unmatched flexibility and accuracy in the study of pollutant dispersion dynamics. Our model subdivides the atmospheric boundary layer (ABL) into distinct sub-layers, facilitating a granular examination of pollutant dispersion dynamics. Each sub-layer is parameterized with specific wind speed profiles and turbulent diffusivity coefficients, adopting their average values. This segmented approach allows for a detailed analysis of vertical and horizontal variations in atmospheric properties, thereby providing a more precise understanding of the mechanisms of pollutant transport and deposition. The key contributions of this work include the development of a generalized analytical model, the incorporation of closed-form solutions, and the meticulous validation of these models through empirical data. By addressing the intricacies of turbulent dispersion and dry deposition, our research offers a comprehensive framework that enhances the predictability and understanding of atmospheric pollutant behavior. In the course of this contribution, we have demonstrated the equivalence between two formulations of the pollutant dispersion problem in the atmospheric boundary layer. The problems  $(\mathcal{PS})$  and  $(\mathcal{P})$  differ in their treatment of the source term: in  $(\mathcal{PS})$ , the source term  $Q \cdot \delta(x) \otimes \delta(y) \otimes \delta(z - H_s)$  is directly integrated into the main differential equation, representing a point source, whereas in  $(\mathcal{P})$ , this term is included in the boundary conditions. The equivalence between  $(\mathcal{PS})$  and  $(\mathcal{P})$  is proven using mollifiers  $(\rho_n)$ , smooth functions that handle the singularity of the source term [11]. The solution obtained not only generalizes but also extends previously established solutions. For a single layer and two-dimensional case, it corresponds to the solutions developed by Kumar [15] and Seinfeld [25]. In the context of multi-layer and three-dimensional scenarios, our model aligns with the solutions provided by Farhane et al. [7] and Marie et al. [19] This demonstrates the robustness and validity of our model across various parameterization conditions, confirming its applicability and accuracy in diverse atmospheric settings. The convergence of the proposed solution is demonstrated through rigorous analysis, showing that a minimal number of eigenvalues are sufficient. This efficiency offers a significant advantage over methods like the Generalized Integral Laplace Transform Technique (GILTT) [28], which often require many more eigenvalues for accuracy. Achieving convergence with fewer eigenvalues ensures both accuracy and computational efficiency, enhancing the model's applicability in real-time atmospheric studies.

Validation against the Hanford experiment data [3] demonstrates the model's accuracy, showing a strong correlation and minimal bias between observed and projected pollutant concentrations. This confirms the model's reliability and statistical robustness. Compared with existing models by Marie et al.[19] and Laouaoucha et al.[16] for cases without deposition, and Moreira et al.[21] and Kumar and Sharan [15] for cases with deposition, our model exhibits superior performance in predicting pollutant dispersion. These findings position our model as a powerful tool for investigating complex environmental phenomena, offering critical insights for both scientific research and practical applications in air quality management. To accomplish the goals of this study, the paper is organized as follows: Section 2 covers the modeling of the advection-diffusion equation. Section 3 explains the construction of the solution and the employed parameterizations. Section 4 showcases the results and provides a statistical performance analysis. Finally, Section 5 concludes the study.

## 2. Atmospheric Pollutant Advection-Diffusion Equation Modeling and Construction of Analytical Solutions

The advection-diffusion equation related to atmospheric pollution is fundamentally expressed as a principle of conservation of suspended particles. This statement is mathematically formalized by the following expression [31]:

$$\frac{Dc_{tot}}{Dt} = \frac{\partial c_{tot}}{\partial t} + \nabla \cdot (\mathbf{U}_{tot} c_{tot}) = S \quad (1)$$

where:

- $\frac{D}{Dt}$ : Represents the substantial derivative, capturing the rate of change in pollutant concentration from the perspective of a moving air parcel, embodying both the temporal and spatial variations due to airflow.
- $C_{tot}$ : Stands for the total concentration of pollutants, which includes both the average concentration and the transient fluctuations attributable to atmospheric turbulence.
- $U_{tot}$ : Denotes the total wind velocity vector represented by  $(U, V, W)^T$ , where  $U$  indicates the east-west component,  $V$  the north-south component, and  $W$  the vertical component, encompassing both the average wind speed and its instantaneous fluctuations.
- $\partial/\partial t$ : Indicates the partial derivative with respect to time, denoting how the concentration of pollutants changes at a fixed point as time progresses.
- $\nabla$ : Is the gradient operator, employed to calculate the spatial gradient of the pollutant concentration.
- $\nabla \cdot (\mathbf{U}_{tot} C_{tot})$ : Describes the divergence of the wind velocity and pollutant concentration product, representing the net movement of pollutants carried by the wind across the spatial domain.
- $S$ : Is the source term within the equation, quantifying the addition or removal of pollutants from the atmosphere via various processes such as industrial emissions, chemical reactions, or the deposition and uptake by terrestrial surfaces and vegetation.

Reynolds decomposition [30] is a pivotal technique for analyzing turbulent flows. It separates the total wind velocity  $\mathbf{U}_{tot}$  and pollutant concentration  $c_{tot}$  into their average components,  $\mathbf{U}$  and  $c$ , and their fluctuating components,  $\mathbf{U}'$  and  $c'$ , respectively. This separation is mathematically represented as

$$\mathbf{U}_{tot} = \mathbf{U} + \mathbf{U}'$$

and

$$c_{tot} = c + c'$$

where the prime notation (') indicates the fluctuating part of the quantity. By doing so, it facilitates the understanding of the complex interplay between the mean flow and the superimposed random fluctuations that characterize turbulent diffusion of contaminants in the atmosphere.

Incorporating the decomposed expressions for  $c_{tot}$  and  $\mathbf{U}_{tot}$ , the advection-diffusion equation 1 is reformulated as:

$$\frac{\partial(c + c')}{\partial t} + \nabla \cdot ((\mathbf{U} + \mathbf{U}')(c + c')) = S$$

Applying the averaging operator across the equation, the mean of the fluctuations alone cancels out, as they are, by definition, zero:

$$\overline{\frac{\partial c'}{\partial t}} = 0, \quad \overline{\mathbf{U}'} = \mathbf{0}, \quad \overline{c'} = 0$$

Expanding the term  $\nabla \cdot (\mathbf{U}c)$ , we get:

$$\nabla \cdot (\mathbf{U}c) = \nabla \cdot (\mathbf{U}c + \mathbf{U}c' + \mathbf{U}'c + \mathbf{U}'c')$$

After averaging, only the terms involving the averages and the term  $\mathbf{U}'c'$  remain:

$$\overline{\nabla \cdot (\mathbf{U}c)} = \nabla \cdot (\mathbf{U}c) + \nabla \cdot \overline{\mathbf{U}'c'}$$

Assembling the mean terms and subtracting the turbulent diffusion term  $\nabla \cdot \overline{\mathbf{U}'c'}$  from the advection term  $\nabla \cdot (\mathbf{U}c)$ , we ultimately derive the advection-diffusion equation for turbulent flow:

$$\frac{\partial c}{\partial t} + \mathbf{U} \cdot \nabla c = -\nabla \cdot \overline{\mathbf{U}'c'} + S$$

This equation now accurately represents the transport and spread of pollutants in a turbulent atmosphere, accounting for the mean motion of the air as well as the chaotic eddies that enhance diffusion.

In atmospheric modeling, the fluctuating wind component, denoted as  $\mathbf{U}' = (u', v', w')^T$ , captures the erratic behavior of air movement. The gradient transport hypothesis, also known as K-theory, elucidates the mechanism by which turbulence drives materials against their concentration gradients. This is mathematically expressed by :

$$\overline{\mathbf{U}'c'} = -\mathbf{K}\nabla c \quad (2)$$

where the eddy diffusivity matrix  $\mathbf{K}$ , defined as  $\text{diag}(K_x, K_y, K_z)$ , incorporates the eddy diffusivity coefficients  $K_x$ ,  $K_y$ , and  $K_z$  for the  $x$ -,  $y$ -, and  $z$ -directions, respectively. This setup enriches our understanding of turbulent diffusion and its impact on the spatial distribution of pollutants.

Furthermore, the equation  $\overline{\mathbf{U}'c'} = \left( \overline{u'c'}, \overline{v'c'}, \overline{w'c'} \right)^T$  accurately models turbulent fluxes, underscoring the model's effectiveness in simulating atmospheric pollutant transport and distribution, and highlights the pivotal role of turbulent diffusion as described by Fick's laws.:

$$\overline{u'c'} = -K_x \frac{\partial c}{\partial x}, \quad \overline{v'c'} = -K_y \frac{\partial c}{\partial y}, \quad \overline{w'c'} = -K_z \frac{\partial c}{\partial z}.$$

Integrating Equation 2 with the mass continuity principle yields the advection-diffusion equation 1, as rigorously documented by [31]:

$$\partial_t c + \mathbf{U} \cdot \nabla c = \nabla \cdot (\mathbf{K} \nabla c) + S \quad (3)$$

In physics and engineering disciplines, the concept of point forces—actions highly localized in both space and time—is a recurrent theme. To mathematically model such phenomena, the Dirac delta distribution is utilized, enabling the precise identification of point sources. For instance, a point source emitting pollutants at a continuous rate  $Q$  at a specific location  $(x_s, y_s, z_s)$  is represented by the source term  $S(x_s, y_s, z_s)$ , formulated as:

$$S(x_s, y_s, z_s) = Q \cdot \delta(x - x_s) \otimes \delta(y - y_s) \otimes \delta(z - z_s),$$

with  $\otimes$  symbolizing the tensor product.

To accurately model the transport of the emitted pollutants, the following boundary conditions are considered:

- (i) The apex of the mixing or inversion layer functions as an impervious boundary preventing the diffusion of contaminants. Consequently, a reflective flux boundary condition is postulated at the height  $H_{mix}$  of the inversion layer, articulated mathematically as:

$$K_z(x, z) \frac{\partial c}{\partial z} = 0, \quad \text{at } z = H_{mix}.$$

- (ii) Addressing the scenario where a pollutant is partially absorbed by the ground surface, Calder [2] delineates an applicable boundary condition in flux terms. It is posited that the ground surface may facilitate partial removal or absorption of the pollutant via deposition, characterized by a deposition velocity  $V_g$ :

$$K_z(x, z) \frac{\partial c}{\partial z} = V_g c, \quad \text{at } z = z_0.$$

where  $z_0$  represents the surface roughness length.

- (iii) The lateral diffusive flux diminishes with increasing distance from the source, approaching zero as  $y$  extends towards the lateral boundary  $L_y$ , formalized by:

$$K_y(x, z) \frac{\partial c}{\partial y} \longrightarrow 0; \quad |y| \longrightarrow L_y,$$

Within the context of this article, key assumptions include:

- The system reaches a state of equilibrium dispersion ( $\partial c / \partial t = 0$ );
- Contributions from  $v(\partial c / \partial y)$  and  $w(\partial c / \partial z)$  are omitted, given that the  $x$ -axis aligns with the mean wind direction, rendering the  $w$  and  $v$  components of wind velocity minor;
- Turbulent diffusion along the mean wind direction is disregarded in comparison to advective transport, implying:

$$u \frac{\partial c}{\partial x} \gg \frac{\partial}{\partial x} \left( K_x \frac{\partial c}{\partial x} \right).$$

These assumptions lead to the steady-state advection-diffusion equation as follows:

$$(\mathcal{PS}) : \begin{cases} u(z) \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} \left( K_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c}{\partial z} \right) + Q \cdot \delta(x) \otimes \delta(y) \otimes \delta(z - H_s); \\ (x, y, z) \in ]0, L_x[ \times ] - L_y, L_y[ \times ]0, H_{mix}[ , \\ \text{Under boundary conditions : } \begin{cases} c(x, y, z) = 0; & x = 0, \\ K_y(x, z) \frac{\partial c(x, y, z)}{\partial y} \rightarrow 0; & |y| \rightarrow L_y, \\ \begin{cases} K_z(x, z) \frac{\partial c(x, y, z)}{\partial z} = V_g c(x, y, z); & z = z_0, \\ K_z(x, z) \frac{\partial c(x, y, z)}{\partial z} = 0; & z = H_{mix}. \end{cases} \end{cases} \end{cases} \quad (4)$$

**Theorem 1.** The problem  $(\mathcal{PS})$  is equivalent to the problem  $(\mathcal{P})$  defined by:

$$(\mathcal{P}) : \begin{cases} u(z) \frac{\partial c}{\partial x} = \frac{\partial}{\partial y} \left( K_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial c}{\partial z} \right); (x, y, z) \in ]0, L_x[ \times ] - L_y, L_y[ \times ]0, H_{mix}[ , \\ \text{Under boundary conditions : } \begin{cases} c(x, y, z) = Q \cdot \delta(x) \otimes \delta(y) \otimes \delta(z - H_s); & x = 0, \\ K_y(x, z) \frac{\partial c(x, y, z)}{\partial y} \rightarrow 0; & |y| \rightarrow L_y, \\ \begin{cases} K_z(x, z) \frac{\partial c(x, y, z)}{\partial z} = V_g c(x, y, z); & z = z_0, \\ K_z(x, z) \frac{\partial c(x, y, z)}{\partial z} = 0; & z = H_{mix}. \end{cases} \end{cases} \end{cases} \quad (5)$$

**Proof of Theorem 1.** The steps for establishing equivalence are outlined as follows:

1. Consider  $c_{\mathcal{P}}(x, y, z)$  as the solution for  $x > 0$  of the system  $(\mathcal{P})$ , and define  $c_{\mathcal{PS}}(x, y, z)$  as follows:

$$c_{\mathcal{PS}}(x, y, z) = \begin{cases} c_{\mathcal{P}}(x, y, z) & \text{for } x > 0, \\ 0 & \text{for } x \leq 0. \end{cases}$$

We will establish that  $c_{\mathcal{PS}}$  satisfies the requirements of system  $(\mathcal{PS})$ .

2. To improve solution regularity, we apply mollifiers  $\rho_n$ , as referenced in [11], over  $]0, +\infty[$ , defined as follows:

$$c_{\mathcal{PS},n}(x, y, z) = c_{\mathcal{PS}}(x, y, z) * \rho_n(x) = \begin{cases} c_{\mathcal{P},n}(x, y, z); & x > 0, \\ 0; & \text{otherwise,} \end{cases} = c_{\mathcal{P},n}(x, y, z) \cdot H(x)$$

with  $c_{\mathcal{P},n}(x, y, z) = c_{\mathcal{P}}(x, y, z) * \rho_n(x)$  and using the Heaviside function  $H(x)$ , which is 1 for  $x > 0$  and 0 otherwise, where  $*$  denotes convolution.

3. We differentiate  $c_{\mathcal{PS},n}$  with respect to  $x$ , leading to:

$$\frac{\partial c_{\mathcal{PS},n}}{\partial x} = \frac{\partial c_{\mathcal{P},n}}{\partial x} \cdot H(x) + c_{\mathcal{P},n} \cdot H'(x) = \frac{\partial c_{\mathcal{P},n}}{\partial x} \cdot H(x) + c_{\mathcal{P},n}(0, y, z) \cdot \delta(x),$$

4. Integrating the advection and diffusion terms, we find:

$$\begin{aligned} u(z) \frac{\partial c_{\mathcal{PS},n}}{\partial x} - \nabla \cdot (K \nabla c_{\mathcal{PS},n}) &= u(z) \frac{\partial c_{\mathcal{P},n}}{\partial x} - \nabla \cdot (K \nabla c_{\mathcal{P},n}) + u(z) c_{\mathcal{P},n}(0, y, z) \cdot \delta(x) \\ &= Q \cdot \delta(x) \otimes \delta(y) \otimes \delta(z - H_s). \end{aligned}$$

This confirms that  $c_{\mathcal{P}}$  corresponds to the system  $(\mathcal{P})$  when  $n$  approaches infinity, thus completing the proof of equivalence between the systems  $(\mathcal{PS})$  and  $(\mathcal{P})$ .

□

The problem  $(\mathcal{P})$  can be transformed into a series of specific advection-diffusion problems defined for each sub-layer of the atmospheric boundary layer, subdivided into  $H$  levels. For each level, the formulations of the turbulent diffusivity coefficients and wind profile adopt average values, as cited in [6]. Furthermore, two boundary conditions are applied at the ABL's extremities, at  $z = z_0$  and at  $H_{mix}$  (the height of the ABL), supplemented by continuity conditions for both the concentration and its flux at the interfaces between sub-layers. These continuity conditions, as shown in Figure 1, are expressed mathematically as follows

- The concentration at the end of a sub-layer must equal the concentration at the beginning of the subsequent sub-layer to ensure the continuity of concentration across sub-layer interfaces, as denoted by the equation

$$c_h = c_{h+1}, \quad \text{for } h = 1, 2, \dots, H-1$$

- The concentration flux, which is the product of diffusivity ( $K_z$ ) and the concentration gradient with respect to the vertical axis ( $z$ ), must also be continuous across the interfaces between sub-layers. This continuity is captured by the equation

$$K_{z,h} \frac{\partial c_h}{\partial z} = K_{z,h+1} \frac{\partial c_{h+1}}{\partial z}, \quad \text{for } h = 1, 2, \dots, H-1.$$

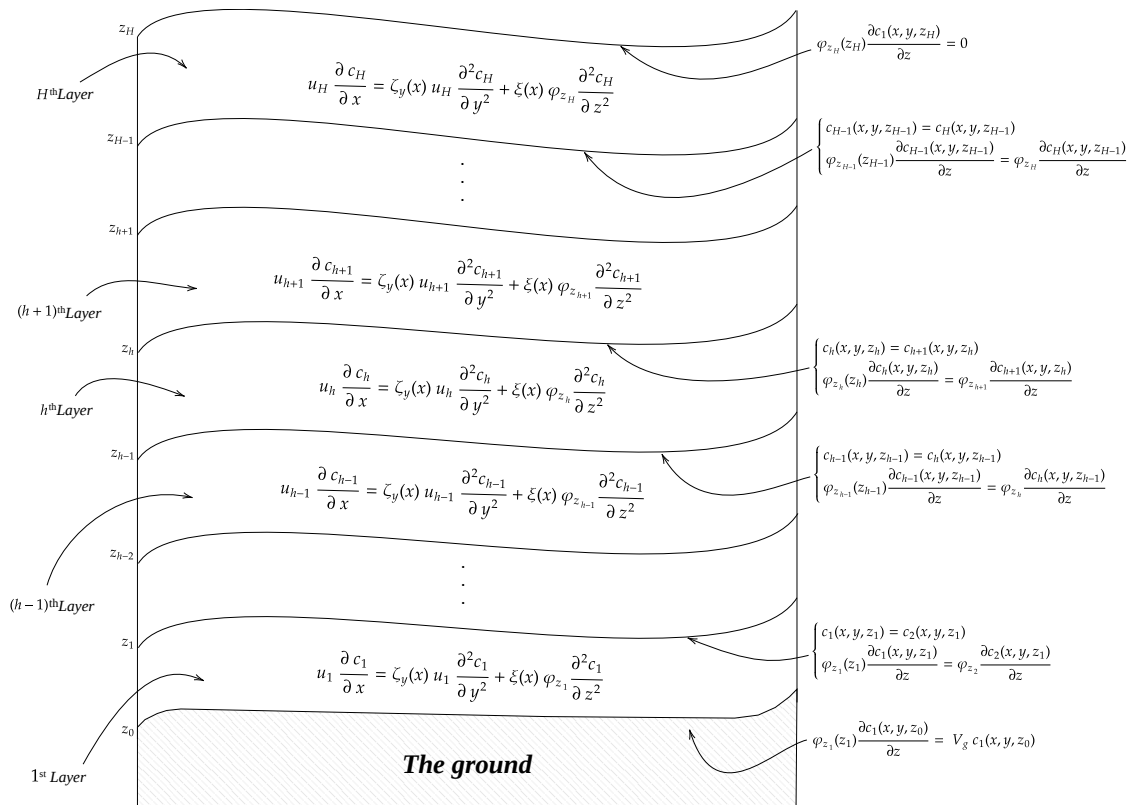
We consider the atmospheric boundary layer's intricate dynamics, where the eddy diffusivities adopt separable formulations that illuminate the interplay between horizontal and vertical mixing processes [7]. Specifically, these formulations are expressed as:

$$K_y(x, z) = \zeta_y(x) u_h, \quad (6)$$

$$K_z(x, z) = \zeta_z(x) \varphi_{z,h}. \quad (7)$$

With this foundation, the equation  $(\mathcal{P}_H)$  outlines the advection-diffusion dynamics across each sub-layer of the atmospheric boundary layer, represented through a set of partial differential equations, expressed as follows:

$$(\mathcal{P}_H) : \left\{ \begin{array}{l} u_h \frac{\partial c_h}{\partial x} = \zeta_y(x) u_h \frac{\partial^2 c_h}{\partial y^2} + \xi(x) \varphi_{z_h} \frac{\partial^2 c_h}{\partial z^2}; (x, y, z) \in ]0, L_x[ \times ] - L_y, L_y[ \times ] z_{h-1}, z_h[ , \\ \forall h \in \{1, \dots, H\} \\ \text{Under the conditions : } \left\{ \begin{array}{l} \varphi_{z_1} \frac{\partial c_1(x, y, z_0)}{\partial z} = V_g c_1(x, y, z_0); \\ c_{h-1}(x, y, z_{h-1}) = c_h(x, y, z_{h-1}) \\ \varphi_{z_{h-1}} \frac{\partial c_{h-1}(x, y, z_{h-1})}{\partial z} = \varphi_{z_h} \frac{\partial c_h(x, y, z_{h-1})}{\partial z} \\ \varphi_{z_H} \frac{\partial c_H(x, y, z_H)}{\partial z} = 0 \end{array} \right. , \forall h \in \{2, \dots, H\}, \end{array} \right. \quad (8)$$



**Figure 1.** Representation of the vertical subdivision of the atmospheric boundary layer into  $H$  sub-layers and the continuity of concentration and flux at the interface of each sub-layer.

**Theorem 2. (Solution to the  $\mathcal{P}_H^{\text{th}}$  Problem)**

The concentration within the  $H^{\text{th}}$  sub-layer, denoted by  $c_H(x, y, z)$ , which is the solution to the problem  $\mathcal{P}_H$ , is given by the following expression:

$$c_H(x, y, z) = \frac{Q}{2\sqrt{\pi \int_0^x \zeta_y(s) ds}} \exp\left(-\frac{y^2}{4 \int_0^x \zeta_y(s) ds}\right) \cdot \left[ \sum_{n=1}^{\infty} \exp\left(-\gamma_n^2 \int_0^x \xi(s) ds\right) P_{H,n}(z) \cdot \left\{ \sum_{h=2}^H P_{h,n}(H_s) + \sqrt{2} \frac{\cos(\lambda_{1,n}(H_s - z_0)) + v_g \sin(\lambda_{1,n}(H_s - z_0))}{\sqrt{u_1(1 + v_g^2)(z_1 - z_0)}} \right\} + \frac{1}{\sum_{h=1}^H u_h(z_h - z_{h-1})} \right] \quad (9)$$

where

$$P_{h,n} = \begin{cases} \frac{1}{\left[\sum_{h=1}^H u_h(z_h - z_{h-1})\right]^{1/2}}; & \text{if } \gamma_n = 0 \\ \frac{\alpha_{h,n} \cos(\lambda_{h,n} z) + \beta_{h,n} \sin(\lambda_{h,n} z)}{\|P_{h,n}\|}; & \text{if } \gamma_n \neq 0 \end{cases} \quad (10)$$

with :

- The coefficient  $\alpha_{h,n}$  is determined by the following relationship:

$$\alpha_{h,n} = \frac{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}}{2\varphi_{z_h} \lambda_{h,n}} \left[ \left( \cos((\lambda_{h,n} + \lambda_{h-1,n})z_{h-1}) + \frac{\varphi_{z_h} \lambda_{h,n} + \varphi_{z_{h-1}} \lambda_{h-1,n}}{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}} \right. \right. \\ \left. \left. \cos((\lambda_{h,n} - \lambda_{h-1,n})z_{h-1}) \right) \alpha_{h-1,n} + \left( \sin((\lambda_{h,n} + \lambda_{h-1,n})z_{h-1}) - \right. \right. \\ \left. \left. \frac{\varphi_{z_h} \lambda_{h,n} + \varphi_{z_{h-1}} \lambda_{h-1,n}}{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}} \sin((\lambda_{h,n} - \lambda_{h-1,n})z_{h-1}) \right) \beta_{h-1,n} \right]; \quad (11)$$

- The coefficient  $\beta_{h,n}$  is determined by the following relationship:

$$\beta_{h,n} = \frac{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}}{2\varphi_{z_h} \lambda_{h,n}} \left[ \left( \sin((\lambda_{h,n} + \lambda_{h-1,n})z_{h-1}) + \frac{\varphi_{z_h} \lambda_{h,n} + \varphi_{z_{h-1}} \lambda_{h-1,n}}{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}} \right. \right. \\ \left. \left. \sin((\lambda_{h,n} - \lambda_{h-1,n})z_{h-1}) \right) \alpha_{h-1,n} - \left( \cos((\lambda_{h,n} + \lambda_{h-1,n})z_{h-1}) - \right. \right. \\ \left. \left. \frac{\varphi_{z_h} \lambda_{h,n} + \varphi_{z_{h-1}} \lambda_{h-1,n}}{\varphi_{z_h} \lambda_{h,n} - \varphi_{z_{h-1}} \lambda_{h-1,n}} \cos((\lambda_{h,n} - \lambda_{h-1,n})z_{h-1}) \right) \beta_{h-1,n} \right]; \quad (12)$$

- The norm  $\|P_{h,n}\|$  is defined as:

$$\|P_{H,n}\|^2 = \sum_{h=1}^H \int_{z_{h-1}}^{z_h} u_h \left( P_{h,n}(s) \right)^2 ds \\ = \sum_{h=1}^H \frac{u_h}{2\lambda_{h,n}} \left[ \sin(\lambda_{h,n}(z_h - z_{h-1})) \left( (\alpha_{h,n}^2 - \beta_{h,n}^2) \cos(\lambda_{h,n}(z_h + z_{h-1})) \right. \right. \\ \left. \left. + 2\alpha_{h,n}\beta_{h,n} \sin(\lambda_{h,n}(z_h + z_{h-1})) \right) + \lambda_{h,n}(\alpha_{h,n}^2 + \beta_{h,n}^2)(z_h - z_{h-1}) \right] \quad (13)$$

- The parameter  $\lambda_{h,n}$  is characterized by the equation:

$$\lambda_{h,n} = \gamma_n \sqrt{\frac{u_h}{\varphi_{z_h}}} \quad (14)$$

with the associated eigenvalues the eigenvalues  $\gamma_n$ , for  $n \in \mathbb{N}^*$ , associated with this problem are real and discrete. Additionally, the corresponding eigenfunctions  $P_{h,n}$  are mutually orthogonal.

**Lemma 1. (Transformed  $\mathcal{P}_H$  Problem Formulation)**

The  $\mathcal{P}_H$  problem, when the Fourier transform is applied to the lateral coordinate  $y$ , is reformulated in terms of the transformed variable  $\chi_h^\omega$ , leading to the subsequent system :

$$\left\{ \begin{array}{l} u_h \frac{\partial \chi_h^\omega}{\partial x} = \zeta(x) \varphi_{z_h} \frac{\partial^2 \chi_h^\omega}{\partial z^2}; (x, z) \in ]0, L_x[ \times ]z_{h-1}, z_h[, \forall h \in \{1, \dots, H\} \\ \text{Under the conditions : } \left\{ \begin{array}{l} \varphi_{z_1} \frac{\partial \chi_1^\omega(x, z_0)}{\partial z} = V_g \chi_1^\omega(x, z_0); \\ \chi_{h-1}^\omega(x, z_{h-1}) = \chi_h^\omega(x, z_{h-1}); \\ \varphi_{z_{h-1}} \frac{\partial \chi_{h-1}^\omega(x, z_{h-1})}{\partial z} = \varphi_{z_h} \frac{\partial \chi_h^\omega(x, z_{h-1})}{\partial z}; \\ \varphi_{z_H} \frac{\partial \chi_H^\omega(x, z_H)}{\partial z} = 0. \end{array} \right. , \forall h \in \{2, \dots, H\} \end{array} \right.$$

where  $\chi_h^\omega(x, z)$  is defined as:

$$\chi_h^\omega(x, z) = \hat{c}_h^\omega(x, z) \cdot \exp\left((2\pi)^2 \omega^2 \int_0^x \zeta_y(s) ds\right) \quad (15)$$

and  $\hat{c}_h^\omega(x, z)$  denotes the Fourier transformation of  $c_h$  with respect to  $y$ , which is given by:

$$\hat{c}_h^\omega(x, z) = \int_{-\infty}^{+\infty} c_h(x, y, z) e^{-2i\pi\omega y} dy, \quad h \in \{1, \dots, H\} \quad (16)$$

**Proof of Lemma 1.** In proving the lemma, we adhere to the following steps:

- We begin by applying the Fourier transform with respect to the lateral coordinate  $y$ , as presented in Eq 16, to the  $\mathcal{P}_H$  problem. The resulting equation is:

$$u_h \left[ \frac{\partial \hat{c}_h^\omega}{\partial x} + (2\pi)^2 \omega^2 \zeta_y(x) \hat{c}_h^\omega \right] = \zeta(x) \varphi_{z_h} \frac{\partial^2 \hat{c}_h^\omega}{\partial z^2}, \quad z \in ]z_{h-1}, z_h[. \quad (17)$$

- We calculate the derivative of  $\chi_h^\omega(x, z)$  with respect to  $x$ , obtaining:

$$\frac{\partial \chi_h^\omega}{\partial x} = \left[ \frac{\partial \hat{c}_h^\omega}{\partial x} + (2\pi)^2 \omega^2 \zeta_y(x) \hat{c}_h^\omega \right] \exp\left((2\pi)^2 \omega^2 \int_0^x \zeta_y(s) ds\right). \quad (18)$$

- We multiply both sides of Eq 17 by the exponential term  $\exp((2\pi)^2 \omega^2 \int_0^x \zeta_y(s) ds)$ . Given that  $u_h$  and  $\varphi_{z_h}$  remain constants within each sub-layer, it simplifies to:

$$u_h \frac{\partial \chi_h^\omega}{\partial x} = \zeta(x) \varphi_{z_h} \frac{\partial^2 \chi_h^\omega}{\partial z^2}, \quad z \in ]z_{h-1}, z_h[ \quad (19)$$

- We apply the same method to the boundary conditions, expressing them in terms of  $\chi_h^\omega$  to ensure consistency with the transformed system.

□

Having established the lemma, we now proceed to employ its results to demonstrate the theorem concerning the solution to the  $\mathcal{P}_H$  problem.

**Proof of Theorem 2.** The construction of the solution for the  $\mathcal{P}_H$  problem unfolds through the following steps:

- Applying the lemma 1, we transform the  $\mathcal{P}_H$  problem into a formulation that depends on  $\chi_h^\omega$ ;

- Representing  $\chi_h^\omega(x, z)$  as a series, we express it in a separated variables form:

$$\chi_h^\omega(x, z) = \sum_{n=0}^{\infty} G_{h,n}^\omega(x) P_{h,n}(z), \quad h \in \{1, \dots, H\}.$$

- Verifying that the functions  $G_{h,n}^\omega$  and  $P_{h,n}$  satisfy their respective differential equations. We must therefore confirm that  $G_{h,n}^\omega$  satisfies the equation

$$\frac{dG_{h,n}^\omega}{dx} + \gamma_n^2 \xi(x) G_{h,n}^\omega = 0, \quad x \in ]0, L_x[ \quad (20)$$

and  $P_{h,n}(z)$  adheres to the system

$$\left\{ \begin{array}{l} \varphi_{z_h} \frac{d^2 P_{h,n}}{dz^2} + \gamma_n^2 u_h P_{h,n} = 0; \quad z \in ]z_{h-1}, z_h[, \quad h \in \{1, \dots, H\} \\ \text{Under the conditions : } \left\{ \begin{array}{l} \varphi_{z_1} \frac{dP_{1,n}(z_0)}{dz} = V_g P_{1,n}(z_0); \\ P_{h-1,n}(z_{h-1}) = P_{h,n}(z_{h-1}); \\ \varphi_{z_{h-1}} \frac{dP_{h-1,n}(z_{h-1})}{dz} = \varphi_{z_h} \frac{dP_{h,n}(z_{h-1})}{dz}; \\ \varphi_{z_H} \frac{dP_{H,n}(z_H)}{dz} = 0. \end{array} \right. , \quad h \in \{2, \dots, H\} \end{array} \right. \quad (21)$$

- Determining the specific forms of  $G_{h,n}$  and  $P_{h,n}$  ensures that they are respectively expressed as:

$$G_{h,n}^\omega(x) = \mu_n(\omega) \cdot \exp\left(-\gamma_n^2 \int_0^x \xi(s) ds\right) \quad (22)$$

where  $\mu_n$  is an arbitrary function depending on  $\omega$ , and

$$P_{h,n}(z) = \alpha_{h,n} \cos(\lambda_{h,n} z) + \beta_{h,n} \sin(\lambda_{h,n} z) \quad (23)$$

where  $\lambda_{h,n}$  is expressed in Eq 14. This formulation must meet the system's criteria, resulting in the determination of  $\alpha_{h,n}$  and  $\beta_{h,n}$ , as specified in Eqs 11 and 12 respectively.

- The continuity condition between sub-layers necessitates a recursion of eigenvalues  $\lambda_{h,n}$  and the eigenfunctions  $P_{h,n}$ , for  $h \in \{1, \dots, H\}$ . This process begins by determining the eigenvalues associated with the first layer,  $\lambda_{1,n}$ , using the conditions related to  $P_{1,n}$ . The resulting expressions are enumerated below:

- The function  $P_{1,n}(z)$  is expressed as:

$$P_{1,n}(z) = \cos(\lambda_{1,n}(z - z_0)) + v_g \sin(\lambda_{1,n}(z - z_0)) \quad (24)$$

where  $v_g = \frac{V_g}{\varphi_{z_1} \lambda_{1,n}}$ .

- The norm of  $P_{1,n}$  is given by:

$$\|P_{1,n}\|^2 = \begin{cases} u_1(z_1 - z_0); & \text{when } \gamma_n = 0 \\ u_1 \left(1 + v_g^2\right) \frac{z_1 - z_0}{2}; & \text{when } \gamma_n \neq 0 \end{cases} \quad (25)$$

The recursive generation of eigenvalues for the intermediate and final layers depends on the known values of the previous layers, in accordance with their respective conditions. This approach makes it possible to construct the associated eigenfunctions, succinctly maintaining continuity between the layers. For further details, please refer to Appendix A.1.

- The Sturm-Liouville theorem [1] allows for the expanded representation of  $\chi_H^\omega$  as:

$$\chi_H^\omega(x, z) = \sum_{n=0}^{\infty} a_n \exp\left(-\gamma_n^2 \int_0^x \xi(s) ds\right) P_{H,n}(z).$$

where the eigenfunctions  $P_{h,n}$  form a complete and mutually orthogonal set. Consequently,  $\chi_H^\omega$  is detailed as above. The coefficients  $a_n$  are determined leveraging the orthogonality of  $P_{h,n}$ , calculated as follows:

$$a_n = \sum_{\ell=1}^H \int_{z_{\ell-1}}^{z_\ell} u_\ell \chi_\ell^\omega(0, z) P_{\ell,n}(z) dz = \begin{cases} \frac{Q}{\sum_{h=1}^H u_h (z_h - z_{h-1})}, & \text{when } \gamma_n = 0 \\ Q \sum_{\ell=1}^H P_{\ell,n}(H_s), & \text{when } \gamma_n \neq 0 \end{cases} \quad (26)$$

- Applying the inverse Fourier transform to  $\chi_H^\omega(x, z)$  from Equation (16), and considering that the inverse transform of

$$\exp\left((2\pi)^2 \omega^2 \int_0^x \zeta_y(s) ds\right)$$

is given by

$$\frac{1}{2\sqrt{\pi \int_0^x \zeta_y(s) ds}} \exp\left(-\frac{y^2}{4 \int_0^x \zeta_y(s) ds}\right),$$

leads to the final expression for the solution  $c_H$  of the problem  $\mathcal{P}_H$ .

□

The Crosswind-Integrated Concentration (CIC) model is a tool for analyzing the dispersion of pollutants in the atmosphere, accounting for the horizontal wind component crucial for pollutant transport. It integrates the concentration across the lateral wind direction,  $y$ , yielding a two-dimensional concentration map along the wind direction ( $x$ ) and crosswind direction ( $z$ ). Mathematically, the CIC,  $c_H^y(x, z)$ , is defined by integrating the pollutant concentration  $c_H(x, y, z)$  over  $y$  from  $-\infty$  to  $+\infty$ . This integration reflects the dispersal of pollutants due to the horizontal wind and assesses their impact in both windward and lateral directions.

**Corollary 1.** The Crosswind-Integrated Concentration (CIC),  $c_H^y(x, z)$ , is equal to  $\chi_H^\omega(x, z)$  as follows:

$$c_H^y(x, z) = Q \cdot \left[ \sum_{n=1}^{\infty} \exp\left(-\gamma_n^2 \int_0^x \xi(s) ds\right) P_{H,n}(z) \cdot \left\{ \sqrt{2} \frac{\cos(\lambda_{1,n}(H_s - z_0)) + v_g \sin(\lambda_{1,n}(H_s - z_0))}{\sqrt{u_1(1 + v_g^2)}(z_1 - z_0)} + \sum_{h=2}^H P_{h,n}(H_s) \right\} + \frac{1}{\sum_{h=1}^H u_h (z_h - z_{h-1})} \right] \quad (27)$$

**Proof.** To confirm the corollary, it suffices to verify the Gaussian integral identity:

$$\int_{-\infty}^{+\infty} \frac{1}{2\sqrt{\pi \int_0^x \zeta_y(s) ds}} \exp\left(-\frac{y^2}{4 \int_0^x \zeta_y(s) ds}\right) dy = 1.$$

□

**Corollary 2.** The solution  $c_H$  for the  $\mathcal{P}_H$  problem encompasses and generalizes the previously established solutions under specific parameterizations:

1. **Single-Layer and Two-Dimensional Solution:**

- (a) For a single layer without discretization, where  $\zeta_y \equiv 1$  and  $\zeta \equiv 1$ , our method yields the solution documented by Kumar [15].
- (b) Transitioning to  $v_g = 0$ ,  $\zeta_y \equiv 1$ ,  $\zeta \equiv 1$ , and  $z_0 = 0$  aligns with the solution documented by Seinfeld [25].

2. **Multi-Layer and Three-Dimensional Solution:**

- (a) Setting  $v_g = 0$  retrieves the solution identified by Farhane et al [7].
- (b) Further simplification to  $v_g = 0$  and  $\zeta \equiv 1$  leads to the solution presented by Marie et al [19].

**Proof.** A detailed proof of this corollary, please refer to the Appendix B. □

**Corollary 3.** In the scenario of a single-layer framework, where  $z_0$  approaches 0 and  $z_1$  extends to  $H_{mix}$ , the Crosswind-Integrated Concentration (CIC),  $c_H^y(x, z)$ , is defined as follows:

$$c_1^y(x, z) = \frac{Q}{\bar{u} H_{mix}} \left[ 1 + \frac{2}{1 + v_g^2} \sum_{n=1}^{\infty} \exp\left(-\frac{(n\pi)^2 \bar{\varphi}_z}{\bar{u} H_{mix}^2} x\right) \left\{ (1 + v_g^2) \cos\left(\frac{n\pi}{H_{mix}}(z - H_s)\right) + (1 - v_g^2) \cos\left(\frac{n\pi}{H_{mix}}(z + H_s)\right) + 2 \sin\left(\frac{n\pi}{H_{mix}}(z + H_s)\right) \right\} \right] \quad (28)$$

where:

- $\bar{u}$  represents the average wind speed over the height of the mixing layer, calculated as

$$\bar{u} = \frac{1}{H_{mix}} \int_0^{H_{mix}} u(s) ds,$$

- $\bar{\varphi}_z$  denotes the average eddy diffusivity over the same height, expressed as

$$\bar{\varphi}_z = \frac{1}{H_{mix}} \int_0^{H_{mix}} \varphi_z(s) ds.$$

**Proof.** To validate the Crosswind-Integrated Concentration (CIC) for a scenario where  $H = 1$  (a single-layer framework), we follow these steps:

1. **Substitute Single-Layer Values into the CIC Equation:** Begin by inserting the conditions of a single-layer setup into the original CIC formula from Eqt (27):

$$c_1^y(x, z) = Q \left[ \frac{1}{u_1(z_1 - z_0)} + 2 \sum_{n=1}^{\infty} \exp\left(-\gamma_n^2 \int_0^x \zeta(s) ds\right) \left\{ \frac{\cos(\lambda_{1,n}(z - z_0)) + v_g \sin(\lambda_{1,n}(z - z_0))}{u_1(1 + v_g^2)(z_1 - z_0)} + \frac{\cos(\lambda_{1,n}(H_s - z_0)) + v_g \sin(\lambda_{1,n}(H_s - z_0))}{u_1(1 + v_g^2)(z_1 - z_0)} \right\} \right]$$

where  $\gamma_n^2 = \frac{(n\pi)^2 \bar{\varphi}_z}{\bar{u}(z_1 - z_0)^2}$ .

2. Apply Limits as  $z_0$  Approaches 0 and  $z_1$  Extends to  $H_{mix}$ : Evaluate the limits to reflect the shift to a single-layer framework that spans the entire mixing height  $H_{mix}$ :

$$\begin{aligned} c_1^y(x, z) &= \frac{Q}{\bar{u}H_{mix}} \left[ 1 + \frac{2}{1 + v_g^2} \sum_{n=1}^{\infty} \exp \left( -\frac{(n\pi)^2 \bar{\varphi}_z}{\bar{u}H_{mix}^2} \int_0^x \xi(s) ds \right) \left\{ \left( \cos \left( n\pi \frac{z}{H_{mix}} \right) + v_g \sin \left( n\pi \frac{z}{H_{mix}} \right) \right) \right. \right. \\ &\quad \left. \left. \cdot \left( \cos \left( n\pi \frac{z}{H_{mix}} \right) + v_g \sin \left( n\pi \frac{z}{H_{mix}} \right) \right) \right\} \right] \\ &= \frac{Q}{\bar{u}H_{mix}} \left[ 1 + \frac{2}{1 + v_g^2} \sum_{n=1}^{\infty} \exp \left( -\frac{(n\pi)^2 \bar{\varphi}_z}{\bar{u}H_{mix}^2} \int_0^x \xi(s) ds \right) \left\{ \left( 1 + v_g^2 \right) \cos \left( \frac{n\pi}{H_{mix}} (z - H_s) \right) \right. \right. \\ &\quad \left. \left. + \left( 1 - v_g^2 \right) \cos \left( \frac{n\pi}{H_{mix}} (z + H_s) \right) + 2 \sin \left( \frac{n\pi}{H_{mix}} (z + H_s) \right) \right\} \right] \end{aligned}$$

□

### 3. Turbulent Parameters in Pollutant Dispersion Modeling

- (a) **Parameterizing the Wind Speed Profile,  $u(z)$ .**

The wind speed profile  $u(z)$  is principally derived using surface layer theory enhanced by Monin-Obukhov (M-O) similarity theory [23]. While traditionally limited to the surface layer, extending the M-O scaling across the entire Atmospheric Boundary Layer (ABL) involves maintaining a constant wind speed profile above this initial layer, ensuring the model's extended applicability and continuity.

Gryning et al. [8] have refined this approach to create a comprehensive wind speed profile applicable over the entire ABL, particularly suited for homogeneous terrain. Their advanced model employs a local mixing length composed of three component scales, leading to a robust formulation that incorporates adjustments for atmospheric stability throughout the entire ABL:

$$u(z) = \frac{u_*}{k} \left[ \ln \left( \frac{z}{z_0} \right) + \frac{bz}{L_{MO}} \left( 1 - \frac{z}{2H_{mix}} \right) + \frac{z}{L_{MBL}} - \frac{z}{H_{mix}} \left( \frac{z}{2L_{MBL}} \right) \right], \quad (29)$$

where  $b = 4.7$  is an empirically determined constant, and  $L_{MO}$ , the Monin-Obukhov length [23], plays a critical role in modeling stability within the boundary layer. The mid-boundary layer length,  $L_{MBL}$ , crucial for stable conditions, is given by:

$$L_{MBL} = \frac{H_{mix}}{2} \left[ \left\{ \left( \ln \left( \frac{u_*}{f_c z_0} \right) - B(\mu) \right)^2 + A^2(\mu) \right\}^{1/2} - \ln \left( \frac{H_{mix}}{z_0} \right) - \frac{bH_{mix}}{2L_{MO}} \right]^{-1},$$

In this formulation,  $f_c$  represents the Coriolis parameter,  $k = 0.4$  is the von Karman constant, and  $A \approx 4.9$  and  $B \approx 1.9$  are resistance law functions, dependent on the stability parameter  $\mu$ . Additionally, Gryning et al. proposed an empirical formula for  $L_{MBL}$  that enhances the model's ability to adapt to various atmospheric stability conditions:

$$L_{MBL} = \frac{u_*}{f_c \left[ -2 \ln \left( \frac{u_*}{f_c z_0} \right) + 55 \right]} \exp \left( \frac{(u_*/f_c z_0)^2}{400} \right).$$

- (b) **Parameterizing the Diffusivity Profiles**

- (b.1) **Vertical Diffusivity:  $K_z(x, z)$**

In atmospheric dispersion models, the parameterization of eddy diffusivity,  $K_z$ , significantly influences model accuracy and performance. Traditionally,  $K_z$  has been modeled

as solely a function of height above the ground,  $z$ . However, recent advancements have extended this parameterization to include the downwind distance  $x$ , recognizing its impact on near-source dispersion dynamics.

An innovative approach by Mooney and Wilson [20] introduced a composite model for  $K_z$ , blending both spatial variables into a single expression:

$$K_z(x, z) = \varphi_z(z) \left[ 1 - \exp\left(-\frac{x}{L_1}\right) \right],$$

where  $\varphi_z$  represents the vertical eddy diffusivity as a function of height, and  $L_1 = u(H_s)\tau(H_s)$  denotes the along-wind length scale. This scale delineates the transition across which diffusivity reaches its extensive field value. Here,  $\tau$  signifies the Lagrangian time scale at the source height, reflecting the turbulence's persistence in the atmosphere.

The parameterization of  $\tau$  at the source height  $H_s$  is given by:

$$\tau(z) = \frac{\varphi_z(z)}{\sigma_w^2},$$

with  $\sigma_w$  representing the vertical turbulent intensity. In stable atmospheric conditions, the formulation for  $\sigma_w$  is:

$$\sigma_w = 1.4u_* \left( 1 - \frac{z}{H_{mix}} \right)^{0.75},$$

demonstrating how stability affects turbulence characteristics.

Mangia et al. [18] further refined  $\varphi_z$  based on local similarity and statistical diffusion theories, resulting in the following relation:

$$\varphi_z(z) = \frac{0.3u_*z(1 - z/H_{mix})}{1 + 3.7z/\Lambda} \quad (30)$$

where  $\Lambda$  represents the local Obukhov length and is expressed as:

$$\Lambda = L_{MO} \left( 1 - \frac{z}{H_{mix}} \right)^{(3\alpha_1/2) - \alpha_2},$$

utilizing constants  $\alpha_1 = 3/2$  and  $\alpha_2 = 1$ , derived from the second-order closure model by Nieuwstadt [22], which accounts for stationary turbulence under a constant cooling rate.

(b.2) **Horizontal Diffusivity:  $K_y(x, z)$**

In the realm of atmospheric dispersion modeling, lateral eddy diffusivity plays a crucial role in determining the spread of pollutants in the crosswind direction. This diffusivity is fundamentally expressed through a relationship that ties it to the wind speed profile and the variance in lateral dispersion:

$$K_y(x, z) = \frac{1}{2}u(z) \frac{d\sigma_y^2(x)}{dx},$$

where  $\sigma_y$  represents the standard deviation of the pollutant's distribution in the lateral or crosswind direction, and is predominantly a function of the downwind distance  $x$ . This formulation underscores the dependency of lateral diffusivity on both the vertical wind speed profile and the rate of change in lateral dispersion as pollutants travel away from the source.

This parameterization, based on the foundational work cited from Huang’s theory [12], encapsulates the dynamic interactions between wind speed and atmospheric turbulence. By integrating the vertical wind profile  $u(z)$  with the derivative of the squared standard deviation  $\sigma_y^2$  with respect to  $x$ , the model effectively captures how lateral diffusion varies with both altitude and distance from the source.

4. Results: Data Analysis and Model Validation

The Hanford experiments provided a valuable dataset to evaluate our Model of Crosswind Dispersion and Deposition Dynamics within the atmospheric boundary layer. These experiments, carried out in May and June of 1983, took place in a semi-arid region of southeastern Washington characterized by largely flat terrain. Detailed documentation of the experiments is available in the work by Doran and Horst [3]. Measurements were taken from six dual-tracer releases positioned at distances of 1100, 200, 800, 1600, and 3200 meters from the release point, under conditions ranging from moderately stable to near-neutral. Notably, the deposition velocity was only evaluated for the three farthest distances. There were six test runs in total, as summarized in the compiled Table 1. Each run had a release duration of 30 minutes, except for the fifth run, which was 22 minutes. The data collected, detailed in Doran et al. [4], were formatted as crosswind-integrated tracer concentrations.

**Table 1.** Micrometeorological data and observed crosswind-integrated concentrations ( $c^y/Q$  ( $10^{-3} \text{ sm}^{-2}$ )) from the Hanford diffusion experiment.

| Run | Date<br>(DD/MM/YY) | $L_{MO}$<br>(m) | $u_*$<br>( $\text{ms}^{-1}$ ) | $H_{mix}$<br>(m) | Distance<br>(m) | $c_{SF_6}^y/Q$<br>( $10^{-3} \text{ sm}^{-2}$ ) | $c_{ZnS}^y/Q$<br>( $10^{-3} \text{ sm}^{-2}$ ) | $V_g(\text{ZnS})$<br>( $10^{-2} \text{ ms}^{-1}$ ) |
|-----|--------------------|-----------------|-------------------------------|------------------|-----------------|-------------------------------------------------|------------------------------------------------|----------------------------------------------------|
| 1   | 18-05-83           | 165             | 0.40                          | 325              | 800             | 3.73                                            | 2.24                                           | 4.21                                               |
|     |                    |                 |                               |                  | 1600            | 2.14                                            | 0.98                                           | 4.05                                               |
|     |                    |                 |                               |                  | 3200            | 1.30                                            | 0.57                                           | 3.65                                               |
| 2   | 26-05-83           | 44              | 0.26                          | 135              | 800             | 12.90                                           | 7.47                                           | 1.93                                               |
|     |                    |                 |                               |                  | 1600            | 9.08                                            | 3.25                                           | 1.80                                               |
|     |                    |                 |                               |                  | 3200            | 7.22                                            | 2.31                                           | 1.74                                               |
| 3   | 05-06-83           | 77              | 0.27                          | 182              | 800             | 5.91                                            | 3.06                                           | 3.14                                               |
|     |                    |                 |                               |                  | 1600            | 3.31                                            | 1.32                                           | 3.02                                               |
|     |                    |                 |                               |                  | 3200            | 1.79                                            | 0.66                                           | 2.84                                               |
| 4   | 12-06-83           | 34              | 0.20                          | 104              | 800             | 20.10                                           | 8.04                                           | 1.75                                               |
|     |                    |                 |                               |                  | 1600            | 13.10                                           | 4.26                                           | 1.62                                               |
|     |                    |                 |                               |                  | 3200            | 9.15                                            | 3.14                                           | 1.31                                               |
| 5   | 24-06-83           | 59              | 0.26                          | 157              | 800             | 10.50                                           | 5.25                                           | 1.56                                               |
|     |                    |                 |                               |                  | 1600            | 8.61                                            | 3.38                                           | 1.47                                               |
|     |                    |                 |                               |                  | 3200            | 6.64                                            | 2.92                                           | 1.14                                               |
| 6   | 27-06-83           | 71              | 0.30                          | 185              | 800             | 13.40                                           | 7.23                                           | 1.17                                               |
|     |                    |                 |                               |                  | 1600            | 6.15                                            | 2.52                                           | 1.15                                               |
|     |                    |                 |                               |                  | 3200            | 3.11                                            | 1.25                                           | 1.10                                               |

Samplers were positioned at angular intervals of 8°, 4°, 4°, 2°, and 3° on concentric circles centered at the release point, with radii corresponding to 100, 200, 800, 1600, and 3200 meters, respectively. Crosswind-integrated concentrations offer significant advantages over individual azimuthal values, as they provide a smoother dataset by integrating over multiple samplers, thereby reducing the impact of minor variations in sampler performance. This method also mitigates issues arising from non-Gaussian crosswind tracer distributions. The terrain had a roughness length of 3 cm. The experiment involved simultaneous releases of two tracers: zinc sulfide (ZnS) as the depositing tracer and sulfur hexafluoride (SF<sub>6</sub>) as the non-depositing tracer, both released from a height of 2 meters. The release points for SF<sub>6</sub> and ZnS were less than 1 meter apart. Table A1 provides the micrometeorological data, including the Monin-Obukhov length (L), friction velocity ( $u^*$ ), and the height of the mixing layer ( $H_{mix}$ ). It also

lists the crosswind-integrated tracer concentrations adjusted for the release rate ( $Q$ ) and the computed effective deposition rates ( $V_g$ ) using the surface depletion method described by Doran and Horst [3].

The ZnS tracer, being a polydisperse aerosol, presented challenges in achieving consistent size distribution estimates. This inconsistency hinders accurate prediction of ZnS deposition rates, as these depend on the mass distribution. The deposition velocity ( $V_g$ ) is critical for model evaluation, but literature estimates of  $V_g$  vary with particle size, atmospheric turbulence, and surface characteristics. Combined with uncertainties in the tracer particle size distribution, this variability complicates accurate prediction of deposition velocity. Since  $V_g$  changes with particle size, both size distribution and deposition velocity vary with downwind distance. An effective deposition velocity ( $V_g$ ) for a given distance incorporates these local variations in  $V_g$  from the source to that distance. For comprehensive details on calculating effective deposition rates and wind velocity, refer to Doran and Horst [3].

#### 4.1. Results and Discussions

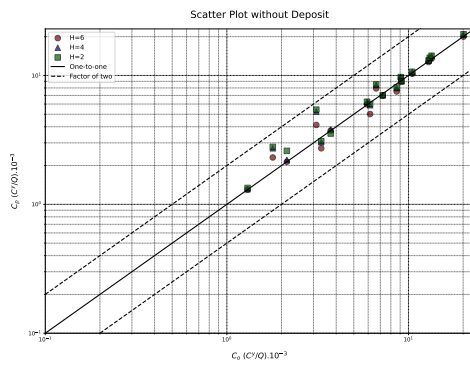
The model was assessed by comparing the crosswind-integrated concentrations of the pollutants ZnS and SF<sub>6</sub> at a height of 1.5 meters above the ground, normalized by the emission rate  $Q$ . The comparison of predicted and observed values is illustrated in Figure 2. The vertical eddy diffusivity was parameterized according to the scheme provided in Eq. (30), while the wind profile followed the formulation described in Eq. (29).

Figure 2 presents scatter plots of predicted versus observed concentrations for the non-depositing material (SF<sub>6</sub>) (Figures (2a) and (2b)) and the depositing material (ZnS) (Figures (2c) and (2d)). Data points located within the outer two dotted lines indicate agreement within a factor of 2, while the central diagonal line represents perfect agreement. It is evident that all simulated concentration data for both the non-depositing material (SF<sub>6</sub>) and the depositing material (ZnS) fall within the dotted lines, indicating a good fit and suggesting that the model is more accurate when deposition processes are included. This contrast between ZnS and SF<sub>6</sub> underscores the significant impact of deposition on model accuracy.

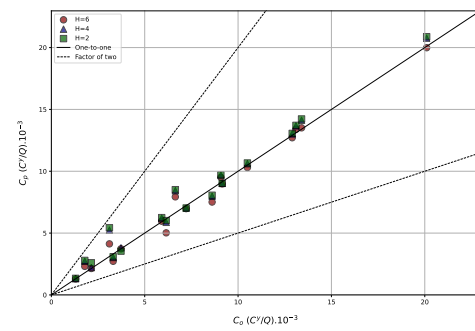
Figures (2a) and (2b) analyze the non-depositing material (SF<sub>6</sub>) using a logarithmic scale and a linear scale, respectively. The logarithmic scale emphasizes lower concentration ranges, providing a more detailed insight into the effects of deposition, while the linear scale offers a straightforward comparison across the entire concentration range. Similarly, Figures (2c) and (2d) present the depositing material (ZnS) using both logarithmic and linear scales, demonstrating the model's consistency and reliability in different deposition scenarios.

The results further demonstrate that increasing the discretization of the model improves the accuracy of predictions. Higher levels of discretization provide a better average representation of the vertical profiles, thereby enhancing the model's capability to predict pollutant dispersion accurately. This improvement is particularly noticeable when comparing predicted and observed values, as the model with higher discretization shows a closer fit to empirical data.

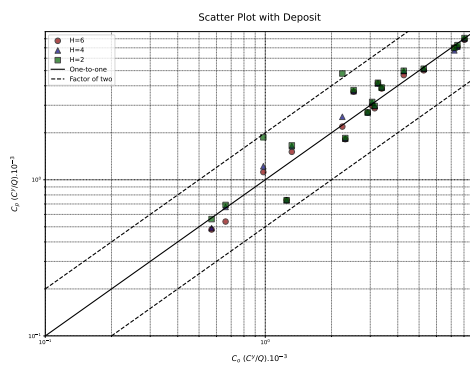
Overall, the analysis reveals that the model performs well in simulating pollutant dispersion, particularly for scenarios involving deposition. The findings emphasize the importance of using appropriate parameterizations and the benefits of higher discretization in improving model accuracy. This comprehensive evaluation underscores the robustness of the model and its potential for reliable predictions in atmospheric pollutant dispersion studies.



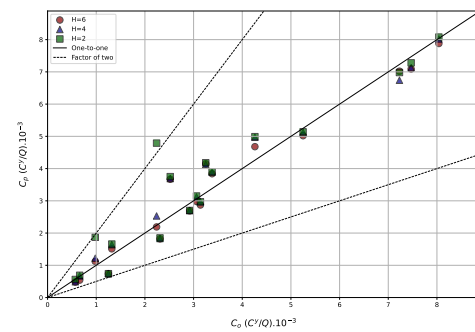
(a) Scatter plot of predicted vs observed concentrations without deposition using a logarithmic scale.



(b) Scatter plot of predicted vs observed concentrations without deposition on a linear scale.



(c) Scatter plot of predicted vs observed concentrations with deposition using a logarithmic scale.



(d) Scatter plot of predicted vs observed concentrations with deposition on a linear scale.

**Figure 2.** Comparative analysis of predicted versus observed concentrations under different deposition conditions, illustrating model performance across a range of environmental settings.

Table 2 presents the performance metrics for models with and without deposition, evaluated using well-established statistical indices. These include NMSE (Normalized Mean Square Error), MRSE (Mean Relative Square Error), COR (Correlation Coefficient), FB (Fractional Bias), FS (Fractional Standard Deviation), MG (Geometric Mean Bias), VG (Geometric Variance), and FAC2 (Factor of Two). These indices provide insights into model accuracy and reliability [14].

For models without deposition ( $V_g = 0$ ), increasing the number of discretization levels  $H$  improves performance. At  $H = 6$ , the model shows very low NMSE and MRSE, high COR, and minimal FB and FS, indicating strong correlation, minimal bias, and variability. When  $H = 4$ , performance slightly decreases but remains high, with low NMSE and high COR. At  $H = 2$ , NMSE and MRSE increase, and COR decreases slightly, but performance is still acceptable. For models with deposition ( $V_g \neq 0$ ), similar trends are observed. Higher  $H$  values result in better performance, with  $H = 6$  showing high COR and low bias. The analysis indicates that all parameterizations simulate observed concentrations well, with NMSE, FB, and FS values close to zero and COR and FAC2 values close to one. Models without deposition generally perform better, but those with deposition also show good performance, particularly with higher discretization levels, demonstrating the model's robustness and accuracy in predicting pollutant dispersion under various conditions.

Table 2 also presents comparisons between the proposed model and previous models by Marie et al. [19] and Laaouaoucha et al. [16] for  $V_g = 0$ , as well as Moreira et al. [21] and Kumar and Sharan [15] for  $V_g \neq 0$ . The results indicate the excellent performance of the proposed solution, as evidenced by the favorable statistical indices across various conditions and discretization levels. This demonstrates

the effectiveness of the proposed model in accurately predicting pollutant dispersion, confirming its superiority and reliability.

**Table 2.** Statistical measures for models with and without deposit.

| Model without Deposit ( $V_g = 0$ ) |         |         |         |          |          |         |        |         |
|-------------------------------------|---------|---------|---------|----------|----------|---------|--------|---------|
| Models                              | NMSE    | MRSE    | COR     | FB       | FS       | MG      | VG     | FAC2    |
| ( $H = 6$ )                         | 0.00591 | 0.00591 | 0.94745 | 0.014    | 0.00710  | 0.99044 | 1.0157 | 1       |
| ( $H = 4$ )                         | 0.00990 | 0.00989 | 0.93503 | −0.04653 | −0.00961 | 0.93302 | 1.0302 | 1       |
| ( $H = 2$ )                         | 0.01142 | 0.01141 | 0.93413 | −0.05485 | −0.00969 | 0.91911 | 1.036  | 1       |
| [19] ( $H = 4$ )                    | 0.08    | -       | 0.86    | −0.02    | 0.05     | -       | -      | 1.0     |
| [19] ( $H = 2$ )                    | 0.1     | -       | 0.82    | 0.1      | 0.04     | -       | -      | 0.92    |
| [16]                                | 0.069   | -       | -       | −0.009   | 0.051    | 0.996   | 1.055  | 1.009   |
| Model with Deposit ( $V_g \neq 0$ ) |         |         |         |          |          |         |        |         |
| Models                              | NMSE    | MRSE    | COR     | FB       | FS       | MG      | VG     | FAC2    |
| ( $H = 6$ )                         | 0.01746 | 0.01746 | 0.94619 | −0.00732 | 0.00877  | 1.0221  | 1.0388 | 1       |
| ( $H = 4$ )                         | 0.02003 | 0.02003 | 0.92379 | −0.02882 | 0.01897  | 0.98231 | 1.0411 | 1       |
| ( $H = 2$ )                         | 0.05188 | 0.05179 | 0.89382 | −0.08679 | 0.01440  | 0.91068 | 1.0962 | 0.94444 |
| [21]                                | 0.09    | -       | 0.95    | −0.22    | −0.08    | -       | -      | 1       |
| [15]                                | 0.088   | -       | 0.96    | −0.196   | 0.32     | -       | -      | 1       |

Figure 3 illustrates the variations in downwind ground-level concentrations for various dry deposition velocities from a source height of 25 meters, as well as the influence of the number of discretizations ( $H$ ) on these concentrations. The sub-figures (3a), (3b), and (3c) correspond to  $H = 2$ ,  $H = 4$ , and  $H = 6$ , respectively.

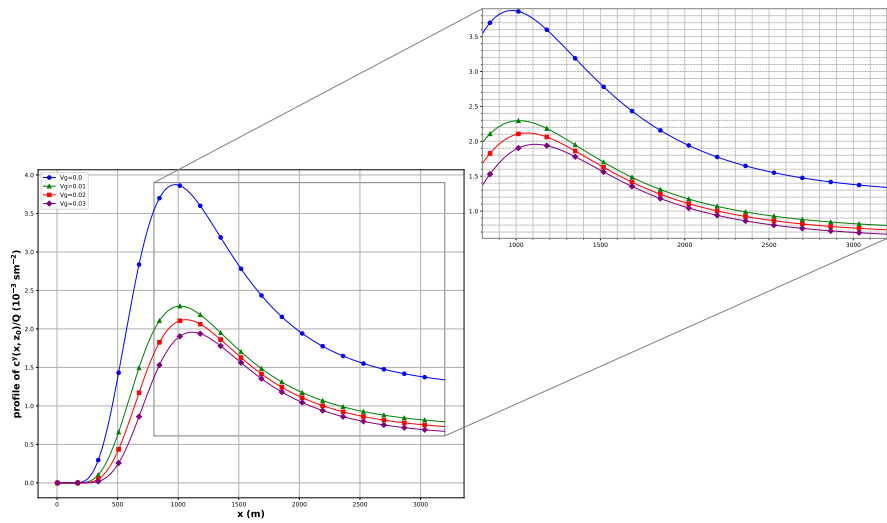
As  $H$  increases, the concentration profiles, both with and without deposition, show improved alignment with the observed data. This improvement is attributable to a more precise representation of wind speed and turbulent diffusivity profiles, thanks to higher levels of discretization. A greater number of layers allows for better capturing of the average characteristics of these profiles.

The profiles show that the highest concentrations occur for contaminants that are completely reflected from the ground. Introducing dry deposition reduces potential human exposure by decreasing airborne concentrations [5]. As dry deposition velocities increase, the location of the peak concentration moves closer to the source. This shift is more evident in the sub-figures as the depletion of pollutants becomes more significant. This behavior is consistent with the predictions obtained using the Gaussian plume model [5].

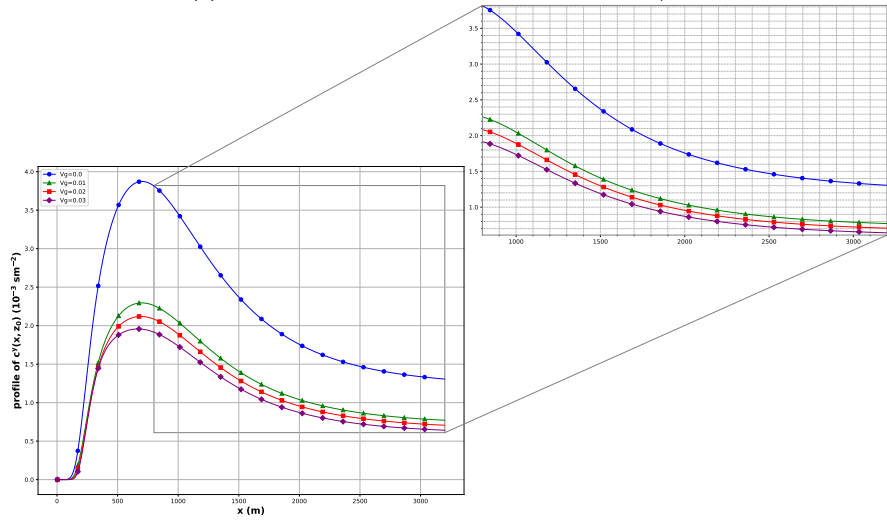
The analysis demonstrates that increasing the number of discretization layers ( $H$ ) enhances the model’s performance in predicting pollutant dispersion. Higher levels of discretization result in a more accurate depiction of vertical profiles, thereby reinforcing the credibility of the model’s predictions. This finding underscores the importance of detailed vertical discretization in atmospheric modeling to achieve accurate and reliable results.

Figure 4 illustrates the numerical convergence of the proposed solution for the concentration as the number of eigenvalues increases, across different values of  $V_g$ . The sub-figures correspond to (4a)  $V_g = 0$ , (4b)  $V_g = 0.01$ , (4c)  $V_g = 0.02$ , and (4d)  $V_g = 0.03$ , each evaluated at three downwind distances ( $x = 800$  m,  $x = 1600$  m, and  $x = 3200$  m). This analysis demonstrates that the solution converges rapidly with the increasing number of eigenvalues.

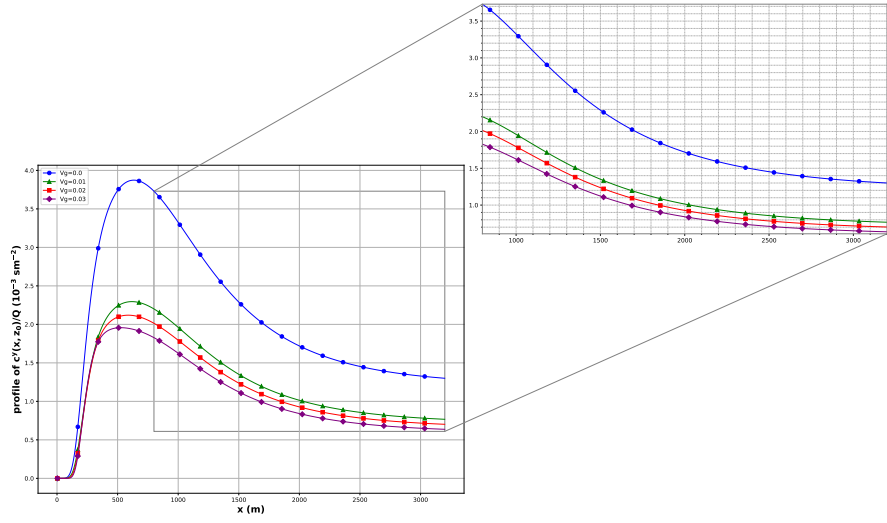
The results confirm that the convergence behavior is consistent across different deposition velocities. The concentration values stabilize after a certain number of eigenvalues, indicating the robustness and efficiency of the proposed solution method. This quick convergence ensures that the model predictions are reliable and can be computed efficiently, even for varying environmental conditions and distances from the source.



(a) Discretization of the ABL into two sub-layers.

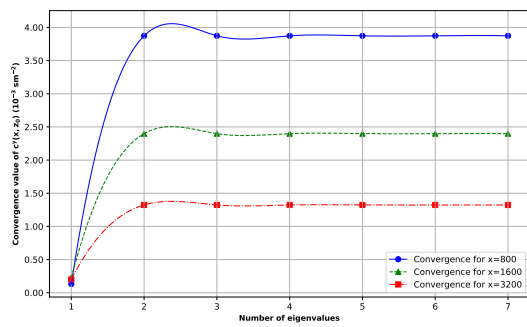


(b) Discretization of the ABL into four sub-layers.

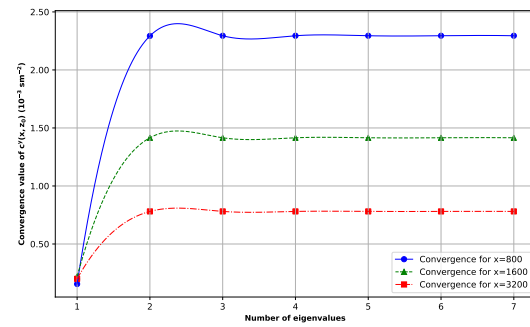


(c) Discretization of the ABL into six sub-layers.

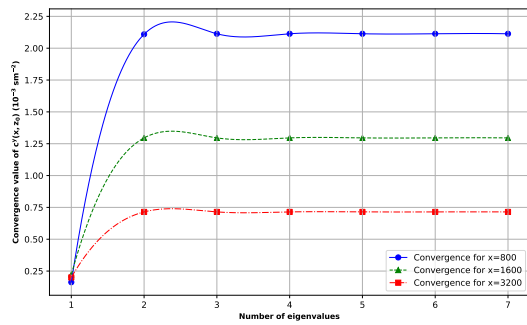
**Figure 3.** Discretization of the ABL into two, four, and six sub-layers, illustrating improved adherence to model parametrizations and closer approximation to experimental measurements with increased discretization.



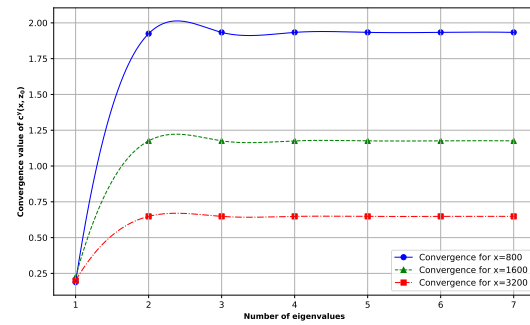
(a) Convergence at  $x = 800$ ,  $x = 1600$ , and  $x = 3200$  m for  $V_g = 0$



(b) Convergence at  $x = 800$ ,  $x = 1600$ , and  $x = 3200$  m for  $V_g = 0.01$



(c) Convergence at  $x = 800$ ,  $x = 1600$ , and  $x = 3200$  m for  $V_g = 0.02$



(d) Convergence at  $x = 800$ ,  $x = 1600$ , and  $x = 3200$  m for  $V_g = 0.03$

**Figure 4.** Analysis of concentration convergence in a discretized ABL model across different distances from the source at  $H_s = 3$  cm, demonstrating the impact of varying deposition velocity  $V_g$ .

## 5. Conclusion

In this study, we developed a comprehensive model for the dispersion of atmospheric pollutants within the boundary layer, incorporating various parameterizations for wind speed profiles, turbulent diffusivity, and dry deposition processes. Our approach subdivides the atmospheric boundary layer into distinct sublayers, enabling a detailed examination of pollutant dispersion dynamics. The analytical solutions obtained were validated against empirical data, demonstrating strong correlation and reliability. The results underscore the model's robustness and accuracy, particularly with higher levels of discretization. This work not only extends existing models but also provides a framework for more precise predictions of pollutant behavior under different atmospheric conditions. Future research could focus on further refining these parameterizations and exploring their applicability in diverse environmental scenarios.

## Abbreviations

The following abbreviations are used in this manuscript:

|     |                                    |
|-----|------------------------------------|
| ABL | Atmospheric Boundary Layer         |
| CIC | Crosswind-Integrated Concentration |

## Appendix A. Construction of the Solution Associated with the First Sub-Layer and Eigenvalue Analysis of the Problem (21).

### Appendix A.1. Construction of the Solution Associated with the First Sub-Layer of the Problem (21)

The solution to Problem (21) is articulated in Eq (23), where  $\alpha_{h,n}$  and  $\beta_{h,n}$  are determined based on the specified conditions for  $h \in \{2, \dots, H\}$ . The continuity conditions establish a recursive relationship between the eigenvalues  $\gamma_n = \lambda_{h,n} \sqrt{\frac{\varphi_{z_h}}{u_h}}$  and the associated eigenfunctions  $P_{h,n}$  for  $h \in \{1, \dots, H\}$ . Initially, the eigenvalues for the first sub-layer (when  $h = 1$ ) must be calculated using the associated condition for  $P_{1,n}$ , which is

$$\varphi_{z_1} \frac{dP_{1,n}(z_0)}{dz} = V_g P_{1,n}(z_0). \quad (A1)$$

Considering the expression for  $P_{1,n}$  as

$$P_{1,n}(z) = \alpha_{1,n} \cos(\lambda_{1,n}z) + \beta_{1,n} \sin(\lambda_{1,n}z), \quad (A2)$$

substituting  $P_{1,n}$ 's expression into the boundary condition yields

$$\alpha_{1,n}(\sin(\lambda_{1,n}z_0) + v_g \cos(\lambda_{1,n}z_0)) - \beta_{1,n}(\cos(\lambda_{1,n}z_0) - v_g \sin(\lambda_{1,n}z_0)) = 0, \quad (A3)$$

where  $v_g = \frac{V_g}{\varphi_{z_1} \lambda_{1,n}}$ .

To satisfy this equation, we can select

$$\begin{cases} \alpha_{1,n} = \cos(\lambda_{1,n}z_0) - v_g \sin(\lambda_{1,n}z_0) \\ \beta_{1,n} = \sin(\lambda_{1,n}z_0) + v_g \cos(\lambda_{1,n}z_0) \end{cases} \quad (A4)$$

which, when substituted into the expression for  $P_{1,n}$ , yields:

$$P_{1,n}(z) = \cos(\lambda_{1,n}(z - z_0)) + v_g \sin(\lambda_{1,n}(z - z_0)). \quad (A5)$$

### Appendix A.2. Eigenvalues Analysis of the Problem (21)

In the analysis of the first sub-layer, the eigenvalues, represented by  $\gamma_n > 0$ , are inferred from the norm of  $P_{1,n}$ . Indeed:

$$\begin{aligned} \|P_{1,n}\|^2 &= \int_{z_0}^{z_1} u_1(P_{1,n}(s))^2 ds \\ &= \frac{u_1}{4\lambda_{1,n}} \left[ 2\lambda_{1,n} \left( 1 + v_g^2 \right) (z_1 - z_0) + \left( 1 - v_g^2 \right) \sin(2\lambda_{1,n}(z_1 - z_0)) \right. \\ &\quad \left. - v_g (\cos(2\lambda_{1,n}(z_1 - z_0)) - 1) \right] \end{aligned} \quad (A6)$$

It is paramount that the norm does not depend on any specific function form. The norm, representing a measure of magnitude or distance, should remain constant across different functions to ensure uniformity and comparability. Therefore, the eigenvalues  $\gamma_n$  are determined under conditions that guarantee this property, leading to:

$$\begin{cases} \sin(2\lambda_{1,n}(z - z_0)) = 0, \\ \cos(2\lambda_{1,n}(z - z_0)) - 1 = 0, \end{cases}$$

which ultimately define the eigenvalues as

$$\lambda_{1,n} = \frac{n\pi}{z_1 - z_0}, \quad n \in \mathbb{N}^*, \quad (\text{A7})$$

yielding a norm expression as follows:

$$\|P_{1,n}\|^2 = u_1(1 + v_g^2) \frac{z_1 - z_0}{2}, \quad n \in \mathbb{N}^*. \quad (\text{A8})$$

For  $n = 0$ , the norm is specifically evaluated considering  $P_{1,0} = 1$  in the designated Eq [A5](#).

Following the complete assessment of eigenvalues for the first sub-layer, our focus shifts to the intermediate and final layers. For the intermediate layers, by implementing the specific condition

$$\begin{cases} P_{h-1,n}(z_{h-1}) = P_{h,n}(z_{h-1}); \\ \varphi_{z_{h-1}} \frac{dP_{h-1,n}(z_{h-1})}{dz} = \varphi_{z_h} \frac{dP_{h,n}(z_{h-1})}{dz}, \end{cases}, \quad h \in \{2, \dots, H\}$$

we arrive at the equation governing the eigenvalues for these layers presented as

$$\begin{aligned} & \varphi_{z_h} \lambda_{h,n} [\alpha_{h,n} \sin(\lambda_{h,n} z_{h-1}) - \beta_{h,n} \cos(\lambda_{h,n} z_{h-1})] \\ & - \varphi_{z_{h-1}} \lambda_{h-1,n} [\alpha_{h-1,n} \sin(\lambda_{h-1,n} z_{h-1}) - \beta_{h-1,n} \cos(\lambda_{h-1,n} z_{h-1})] = 0. \end{aligned}$$

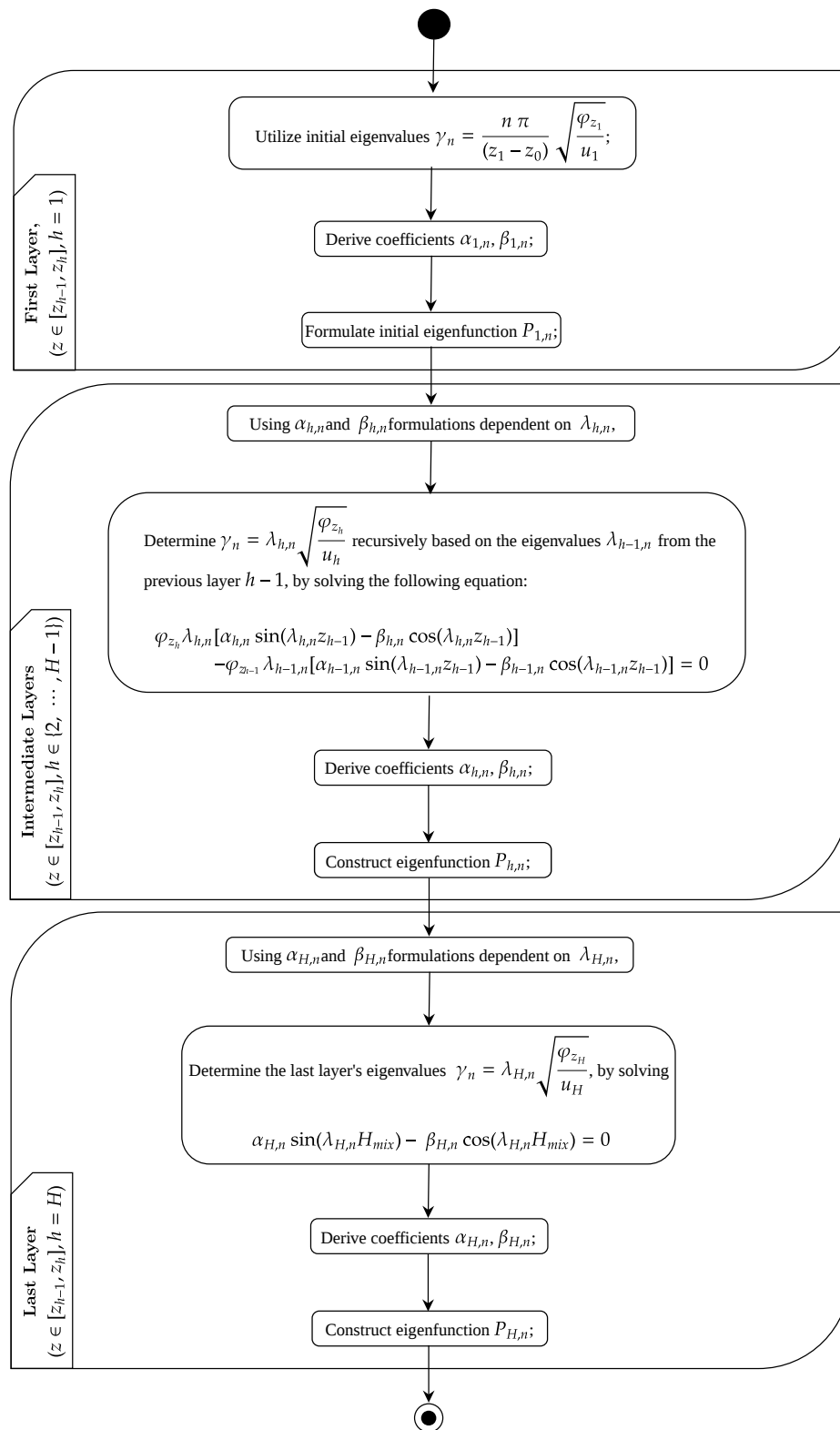
Regarding the last layer, employing the relevant condition

$$\varphi_{z_H} \frac{dP_{H,n}(z_H)}{dz} = 0$$

leads to the formulation of the equation that yields the eigenvalues for this ultimate layer as

$$\alpha_{H,n} \sin(\lambda_{H,n} H_{mix}) - \beta_{H,n} \cos(\lambda_{H,n} H_{mix}) = 0.$$

To facilitate a clear understanding of the eigenvalue generation process for each sub-layer, the accompanying flowchart [A1](#) concisely outlines the analytical steps involved, capturing the recursive determination of eigenvalues and the construction of eigenfunctions as discussed.



**Figure A1.** Flowchart of the Process for Calculating Eigenvalues and Eigenfunctions in the Subdivided Media of the Atmospheric Boundary Layer.

## Appendix B. Derivation of Specific Solutions for $c_H$

In the special case where  $v_g = 0$ , the eqt (9) simplifies to yield the solution as determined by Farhane et al[7], defined by:

$$c(x, y, z) = \frac{1}{2\sqrt{\pi \int_0^x \zeta_y(s) ds}} \exp\left(-\frac{y^2}{4 \int_0^x \zeta_y(s) ds}\right) \sum_{n=0}^{\infty} a_n \exp\left(-\gamma_n^2 \int_0^x \zeta(s) ds\right) P_{H,n}(z).$$

Were, the coefficients  $a_n$  are as defined in eqt (26). Further analysis, with  $\zeta_y \equiv 1$ , leads to a solution analogous to that provided by Marie et al[19].

Transitioning to two dimensions and employing the CIC model, for a single layer we utilize the boundary condition at the top of the atmospheric boundary layer, specifically  $\varphi_{z_H} \frac{dP_H(x, z_H)}{dz} = 0$ . This condition derives the parameters  $\alpha_{H,n} = \cos(\lambda_{1,n} H_{mix})$  and  $\beta_{H,n} = \sin(\lambda_{1,n} H_{mix})$ , leading to the expression  $P_{H,n} = \cos(\lambda_{H,n}(z - H_{mix}))$ . The norm of  $P_{H,n}$  is then given as:

$$\|P_{H,n}\|^2 = \frac{(H_{mix} - z_0)}{2} \left[ 1 + \frac{\sin(2\lambda_{H,n}(H_{mix} - z_0))}{2\lambda_{H,n}(H_{mix} - z_0)} \right],$$

matching the solution identified by Kumar [15].

For Seinfeld's solution[25], we have:

$$\begin{aligned} c_1^y(x, z) &= \frac{Q}{u_1(z_1 - z_0)} \left[ 1 + 2 \sum_{n=1}^{\infty} \exp\left(-\frac{(n\pi)^2 \varphi_{z_1}}{u_1(z_1 - z_0)^2} x\right) \cos(\lambda_{1,n}(z - z_0)) \cos(\lambda_{1,n}(H_s - z_0)) \right] \\ &\stackrel{z_0 \rightarrow 0}{=} \frac{Q}{u_1 z_1} \left[ 1 + 2 \sum_{n=1}^{\infty} \exp\left(-\frac{(n\pi)^2 \varphi_{z_1}}{u_1 z_1^2} x\right) \cos(\lambda_{1,n} z) \cos(\lambda_{1,n} H_s) \right] \\ &\stackrel{z_1 \rightarrow H_{mix}}{=} \frac{Q}{u_1 H_{mix}} \left[ 1 + 2 \sum_{n=1}^{\infty} \exp\left(-\frac{(n\pi)^2 \varphi_{z_1}}{u_1 H_{mix}^2} x\right) \cos\left(\frac{n\pi}{H_{mix}} z\right) \cos\left(\frac{n\pi}{H_{mix}} H_s\right) \right] \end{aligned}$$

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