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PLUMES2.0$_{v1}$– Dilution Model

Update with carbonate chemistry and dissolved oxygen kinetics - Model Theory and User Manual

Model update developed through a grant from
the *Climate Works Foundation*

December 2025

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University of Washington, Office of Sponsored Research
Grant No. GR033216

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Dr. Walter Frick of US EPA (retired), the developer of Visual Plumes, kindly provided us with the UM3 model code written in Pascal, which provided the foundation for developing the Fortran version of UM3 implemented in the PLUMES2.0 code.

PLUMES2.0v1 update represents the next phase of continuing development and enhancement of PLUMES2.0. It includes carbonate chemistry calculations that were made possible through a grant from the ClimateWorks Foundation. Simplified DO/BOD kinetics were added by the developers at SSMC as an added feature in support of water quality compliance assessments. Further improvements will be undertaken based on user community needs and availability of funding support.

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Acronyms and Abbreviations

AMZ	Acute Mixing Zone
BOD	Biochemical oxygen demand
CORMIX	A dilution model originally developed by Cornell University with EPA support.
CMZ	Chronic Mixing Zone
CSTR	Continuously stirred tank reactor
DIC	Dissolved inorganic carbon
DKHW	A multiport dilution model in the VP package based on original technical developments by **D**avis, **K**annberg, and **H**irst in the 1970s (**W**indows based)
DO	Dissolved Oxygen
FRFIELD	Far-field dilution model in the VP package based on Brooks' Laws
FVCOM	Finite Volume Community Ocean Model – a 3D hydrodynamic model
FVCOM-ICM	Salish Sea Model biogeochemical component based on CE-QUAL-ICM
GUI	Graphical User Interface
IDOD	Immediate dissolved oxygen demand
JETLAG	A Lagrangian dilution model of Lee et. al., from the University of Hong Kong
LCV	Lagrangian Control Volume
NPDES	National Pollution Discharge Elimination System
NRFIELD	**R**oberts, **S**nyder, and **B**aumgartner (RSB) dilution model in VP package
ORD	Office of Research and Development
PDSW	**P**rych, **D**avis, and **S**hirazi 3D plume model for **W**indows in VP package with the ability to accommodate surface discharge.
PLUMES	USEPA recommended package of dilution models for effluent discharges.
QA	Quality assurance
QAPP	Quality Assurance Project Plan
QC	Quality control
RMZ	Regulatory Mixing Zone
SSMC	The *Salish Sea Modeling Center* at University of Washington
TA	Total alkalinity
UM3	Three-dimensional version of UMERGE model which is part of the VP package.
UMERGE	A two-dimensional effluent dilution model with plume merging
US EPA	United States Environmental Protection Agency
VP	Visual Plumes
ZID	Zone of Initial Dilution for a typical effluent plume

Executive Summary

The ability to conduct dynamic effluent fate and transport using standalone public domain software with a graphical user interface (GUI) is a core need of the National Pollutant Discharge Elimination System (NPDES) program. Wastewater discharge permits under the NPDES program are designed using effluent mixing and dilution calculations to ensure that the receiving water quality will not be impaired. Visual Plumes (Frick et al., 2004) was a Windows and Pascal based computer application that provided the necessary tools for the required analysis of effluent fate and transport. Visual Plumes had previously superseded the DOS and Fortran based PLUMES (Baumgartner, Frick, and Roberts, 1994) mixing zone modeling system. Visual Plumes simulated single and merging submerged plumes in arbitrarily stratified ambient flow from buoyant submerged as well as surface discharges. Among its features were multiple dilution models, tidal pollutant build-up estimation, a sensitivity analysis capability, and a multi-stressor pathogen decay model. Visual Plumes offered a suite of dilution models including DKHW and UM3 models that are based on the original UDKHDEN and UM models (Muellenhoff et al., 1985), the surface discharge model PDS (Davis, 1999), the NRFIELD model based on RSB (Roberts et al., 1989 a,b,c) and the passive far-field transport and dilution of the wastefield using Brooks' laws (Brooks, N.H., 1969). The most widely used sub-model by default was UM3. Walter E. Frick, formerly from the U.S. Environmental Protection Agency (U.S. EPA) Office of Research and Development (ORD), was the last lead on Visual Plumes. Dr. Frick has since retired, and the Visual Plumes software became incompatible with the current version of the Windows operating system.

As part of unrelated U.S. EPA funded research at the Pacific Northwest National Laboratory and Salish Sea Modeling Center (SSMC) at the University of Washington, a three-dimensional Lagrangian approach-based plume model (FVCOM-plume) was developed (Premathilake and Khangaonkar, 2019). The FVCOM-plume model written in Fortran includes an initial dilution module based on UM3 formulation. That imbedded initial dilution module accommodates multiport diffusers and its performance has been confirmed against Visual Plumes (UM3).

Subsequently, the U.S. EPA, in collaboration with SSMC scientists, initiated this effort towards developing updated model software for simulating dilution of effluent from submerged outfalls. The overall goal was to develop, test, and release the new version of dilution modeling software (renamed PLUMES2.0) along with a User's Manual to U.S. EPA and the user community for distribution. This release and the User's Manual represent the completion of Phase 1 of the development and testing of the software. Additional features and models may be added in subsequent phases based on user community response and needs. In PLUMES2.0, the initial dilution of the effluent, consisting of jet and buoyancy induced dynamic mixing of the effluent plume in the near-field is computed using the UM3 methodology. PLUMES2.0 then allows for analysis of plume fate following stabilization of the wastefield at the trapping depth when it is carried away by the ambient currents and further diluted by turbulence. This far-field transport of the wastefield and dilution is computed using Brooks laws (Brooks, N.H., 1969). Specifically, PLUMES2.0 includes (a) UM3 - initial dilution model, (b) Brook's Far-field model, and (c) a GUI. The associated Model Theory and User Manual (this document), provides basic theory of effluent mixing and dilution principles, concept of mixing zones, and guidance for model use which may range from NPDES permitting to wastewater outfall diffuser design. The document includes step-by-step instructions for setting up the input files and is suitable for new users.

1.0 Introduction

1.1 Background

Wastewater from industrial and municipal facilities may contain pollutants that pose an ecological and/or human health risk. In recognition of the fact that natural mixing causes the concentration of pollutants to diminish in the receiving waters, regulatory agencies allow mixing zones in evaluating water quality compliance and exposure risk. A mixing zone is defined as a small region near the outfall where certain water-quality criteria can be exceeded as long as (a) there is no lethality to the organisms passing through the mixing zone, (b) there are no significant risks to human health, and (c) the designated and existing uses of the water body are not impaired (US EPA, 1991). Effluent discharges and mixing zones are authorized through the Clean Water Act: Section 402 (40 CFR Part 122) National Pollution Elimination System (NPDES) Permits. Water quality compliance for carcinogens and highly toxic substances is typically evaluated at the end of pipe. But for many pollutants, compliance is evaluated at the mixing zone boundaries after the completion of initial rapid mixing and dilution of the effluent with the surrounding waters. The allowable dimensions of mixing zones vary from state to state based on requirements in state water quality standards.

When two fluids carrying the same constituent but at different concentrations mix, the resultant concentration of the mixture is simply the volume averaged concentration. For example, if a concentrated effluent volume V_e (m^3) at a concentration C_e (mg/L) is mixed with a volume V_a of clean water, the resulting concentration C_f after mixing may be simply expressed as $C_f = \frac{C_e}{D}$, where D is the volumetric dilution factor expressed as $D = \frac{(V_e+V_a)}{V_e}$ assuming that ambient concentration C_a is zero. The effluent concentration after mixing is therefore regarded as being reduced by the dilution factor.

In realistic settings, however, the ambient concentration is rarely zero. It must be accounted for to assess compliance with regulations. To do so, the concentration of the effluent constituent of concern is compared against the applicable water quality standard(s) $C_{wqs,}$ after the completion of the dilution process within the allocated mixing zone. The constituent concentration in the water outside the mixing zone must remain below C_{wqs}. Water quality standards for protection of aquatic life are defined based on acute and chronic effects based on duration of exposure. Aquatic organisms can endure exposure to higher concentrations or acute exposure for a short duration of time (e.g., 1 hr). Under chronic exposure (e.g., 96 hrs), lower concentrations can cause ecological impacts. Depending on the applicable water quality regulations, there may be two mixing zone boundaries to consider, (a) Acute Mixing Zone (AMZ) and (b) the Chronic Mixing Zone (CMZ), also known as the Regulatory Mixing Zone (RMZ). Dimensions of these mixing zones vary based on site specific conditions and are explicitly defined in the NPDES permit for the discharge. The estimation of effluent dilution over time and space is necessary for the application of a mixing zone in permit limit derivations and/or the design of an outfall structure/location to achieve a target dilution.

The effluent concentrations following dilution and mixing may be computed using the simple equation below.

$$C_f = \left(\frac{C_e - C_a}{D}\right) + C_a \tag{1}$$

where C_f = Final concentration (mg/L) of the effluent after dilution and mixing with the ambient water,

C_e = Effluent concentration (mg/L) of the discharge or end-of-pipe concentration,
C_a = Ambient or receiving water concentration (mg/L), typically upstream from the discharge, and
D = the Dilution ratio.

In a continuously stirred tank reactor (CSTR) laboratory setting with a known volume(s) the dilution factor D may be estimated in a straightforward manner as the ratio of total volume of the mixed fluid in the reactor to the effluent volume added. In a CSTR, the volumes are fixed and mixing of the two fluids and diffusion process is assumed to have reached completion. In a realistic setting however, computing the volumes of the respective fluids and extent of diffusion is complex and requires the assistance of numerical models or physical dye studies. The process of mixing and dilution itself occurs in the timescale order of minutes and often reaches a steady state within a short distance from the outfall. It is dependent on multiple physical parameters controlled by effluent characteristics such as flow rate, effluent density, outfall port/diffuser dimensions and depth, and receiving water stratification and currents. Upon exiting the outfall, the effluent undergoes rapid mixing due to nearfield momentum (jet) and buoyancy effects. Following this initial dilution, the plume stabilizes at the surface or at a neutrally buoyant trapping depth. The wastefield is then carried away by ambient currents over a longer timescale. The dilution continues to increase gradually during this farfield passive mixing phase from natural turbulence and currents further reducing the concentration of the effluent in the plume. Concentrations and dilution vary throughout the plume downstream of the discharge point.

Accurate determination of D at the specified mixing zone boundary (or C_f in the plume and at the specified mixing zone location) becomes an important requirement for various regulatory needs such as (a) Reasonable Potential Analysis – to evaluate if a constituent detected in effluent has a reasonable potential to exceed water quality criteria, (b) Assessment of compliance with applicable water quality standard based on discharge monitoring data, and (c) computation of Water Quality-based Effluent Limitations (WQBELs). Similarly, the design of diffusers and siting of outfalls for existing or new discharges requires iterative dilution ratio computations as part of feasibility and final design. These assessments require a predictive dilution model.

1.2 Brief history and Overview of Dilution Models

Development of mathematical models to predict mixing and dilution of effluent from wastewater outfalls dates back to early 1950s. Researchers applied principles of continuity, momentum, and energy conservation, integrated using Gaussian principles to study the spreading of buoyant plumes in uniform and stratified but stagnant environments (Rouse et al., 1952; Priestly and Ball, 1955). Numerous studies improved on this early work through the addition of concepts, such as an entrainment function based on local length scales (Morton et al., 1956), port orientation effects (Abraham, 1963; Fan, 1967), and effects of ambient currents and cross flow (Chu, 1979; Wright, 1984). Studies of plumes from multi-port diffusers have included line diffusers (fully merged plumes) in stagnant ambient waters (Pearson, 1956), and experimental laboratory work on merging of plumes (Liseth, 1970, 1976). Subsequently in the 1970s several mathematical models were proposed to simulate buoyant plume discharges varying from single to multiport diffusers, and, mixing in uniform confined environments to stratified flowing conditions (Koh and Fan, 1970; Cederwall, 1971; Sotil, 1971; Kannberg and Davis, 1977; Roberts, 1977; Roberts, 1979 a,b). By the early 1980s, there were numerous mathematical models available from various researchers, each specializing in different aspects of the plume dilution phenomena. Although multiple literature review papers had been published by then (Davis and Shirazi, 1978; Roberts, P.J.W., 1983, 1984, 1985), consolidation of the existing research and models into practical tools along with clear instructions on their use in practice for outfall design or for regulatory analysis did not exist until the mid-1980s.

The need for such guidance became more urgent when US EPA adopted regulations implementing Section 301(h) of the Clean Water Act (PL 97-117) (US EPA, 1982). Under these rules, publicly owned municipal wastewater could be discharged using treatment levels less effective than secondary treatment, after demonstrating compliance with water quality standards at the prescribed "zone of rapid mixing" or the zone of initial dilution (ZID). The demonstrations of environmental acceptability by the NPDES applicants and review by the permit writers required the use of plume models. To ensure consistency in the use of available tools, and quality assurance, EPA provided procedures for calculating the initial dilution and for describing the zone of initial dilution near a discharge site, using five leading dilution models (Muellenhoff et al. 1985). The models were UPLUME, UOUTPLM, UMERGE, UDKHDEN, and ULINE, based on prior work by Teeter and Baumgartner (1979) and Roberts (1977, 1979b). These were codes written in Fortran with differences in their computational approaches but utilized a universal input file format and structure that offered users consistency in input parameters (effluent, diffuser, and receiving water characteristics) and results (plume characteristics including location, size, and flux averaged plume dilution as a function of distance from the outfall). These estimates were based on a Gaussian distribution of concentrations within a plume cross section. The computations stopped at the completion of initial rapid mixing phase, typically after the plume reached the surface or stabilized at a neutrally buoyant trapping depth, thereby defining the ZID.

Most plume models use simplifying assumptions in defining the discharge configuration and the mixing processes (e.g., Gaussian distribution of plume concentration across the plume width, diffusers with simple geometries, and domains with no bounding constraints). In realistic settings, the plume-behavior may be affected by boundary effects (bottom or bank attachment, plume stability), and complex diffuser geometries such that simplifying assumptions in plume models may no longer be valid. Dye studies or laboratory studies involving hydraulic scale models with precise representation of the site-specific conditions may be needed to accurately estimate the initial dilution process. With an emphasis on the importance of boundary interactions on the stability of the plume and mixing processes, Cornell University with support from US EPA developed the CORMIX model. CORMIX consists of a series of software systems for the analysis, prediction, and design of discharges with emphasis on the role of boundary interaction to predict steady state mixing behavior and plume geometry. It classifies momentum and buoyancy of the discharge in relation to boundary interactions to predict mixing behavior. Boundary interactions can be surface or bottom contact or terminal layer formation in density stratified ambient waters. CORMIX was released as a knowledge and inference based expert system package consisting of CORMIX1 (Doneker and Jirka, 1990) for single port discharges, CORMIX2 (Akar and Jirka, 1992) for multiport diffusers, and subsequently CORMIX3 (Jones et al., 1996) for surface discharges.

In 1991, US EPA issued technical guidance for assessing and regulating discharge of toxic substances to the waters of the United States in NPDES permits. This *Technical Support Document for Water Quality Based Toxics Control* (US EPA 1991) was comprehensive and included language about regulatory mixing zones. The guidance was then adopted by various states to develop their own standard procedures for conducting Mixing Zone Studies including the use of dilution models for conducting water quality compliance evaluations. In response to a growing demand and adapting to PC based computing platforms, US EPA released DOS Plumes (Baumgartner et al., 1994) which only included the UM model, an updated version of UMERGE, and RSB, an updated version of ULINE based on experimental studies on multiple 'T' shaped port diffusers (Roberts et al. 1989 a,b,c). DOS Plumes also incorporated the flow classification scheme of the CORMIX model (Jirka and Hinton, 1992), with recommendations for model usage. DOS Plumes and CORMIX then became the two US EPA-supported models for dilution modeling and mixing zone analyses.

DOS Plumes was subsequently upgraded to Visual Plumes (Frick et al., 2004), a Windows-based application that included graphics, time-series input files, user specified units, a conservative tidal background-pollutant build-up capability, a sensitivity analysis capability, and a multi-stressor pathogen decay model that predicts coliform mortality based on temperature, salinity, solar insolation, and water column light absorption. It also included DKHW model that is based on UDKHDEN (Muellenhoff et al., 1985), the surface discharge model PDS (Davis, 1998), the three-dimensional UM3 model based on UM, and the NRFIELD model based on RSB. Visual Plumes was distributed by US EPA. Similarly, the DOS-based CORMIX suite of models were upgraded to a Windows-based application, licensed and distributed by MixZon, Inc. For nearly 15 years since their release, Visual Plumes and CORMIX were the two leading modeling systems that were used extensively by the community for outfall design, siting studies, and mixing zone analyses. Following the release of Windows 10, however, Visual Plumes lost its compatibility with the PC operating system. The community has since primarily relied on CORMIX as the only model readily available to the plume modeling community.

The PLUMES2.0 project provides renewed access to key sub-models of the Visual Plumes model suite.

2.0 Theory and Model Formulation

2.1 Approach and Conceptual Framework

PLUMES2.0 directly adopts the analytical modeling framework that was used in the UM3 model. UM3 in turn is based on the most recent and established theoretical treatment of effluent plumes developed over several decades of research described in Section 1.2 (e.g., Akar and Jirka, 1991; Baumgartner et al., 1994; Brooks, 1960; Fan, 1967; Fischer et al., 1979; Muellenhoff et al., 1985). The conceptual model of a buoyant effluent plume consists of three phases or regimes of physical mixing of two fluids, as shown in Figure 1. The plume dynamics in the immediate vicinity of the diffuser are controlled by jet mixing where effluent is discharged to the ambient waterbody under hydraulic pressure. The jet mixing occurs through momentum flux and turbulent shear accompanied by a drop in pressure. This is followed by a buoyancy-induced transition phase including interaction with ambient currents. The final phase is the farfield passive transport phase where stabilized wastefield is carried away by ambient currents and further mixed with surrounding waters through spreading due to combination of remnant buoyancy and natural turbulence in the receiving water.

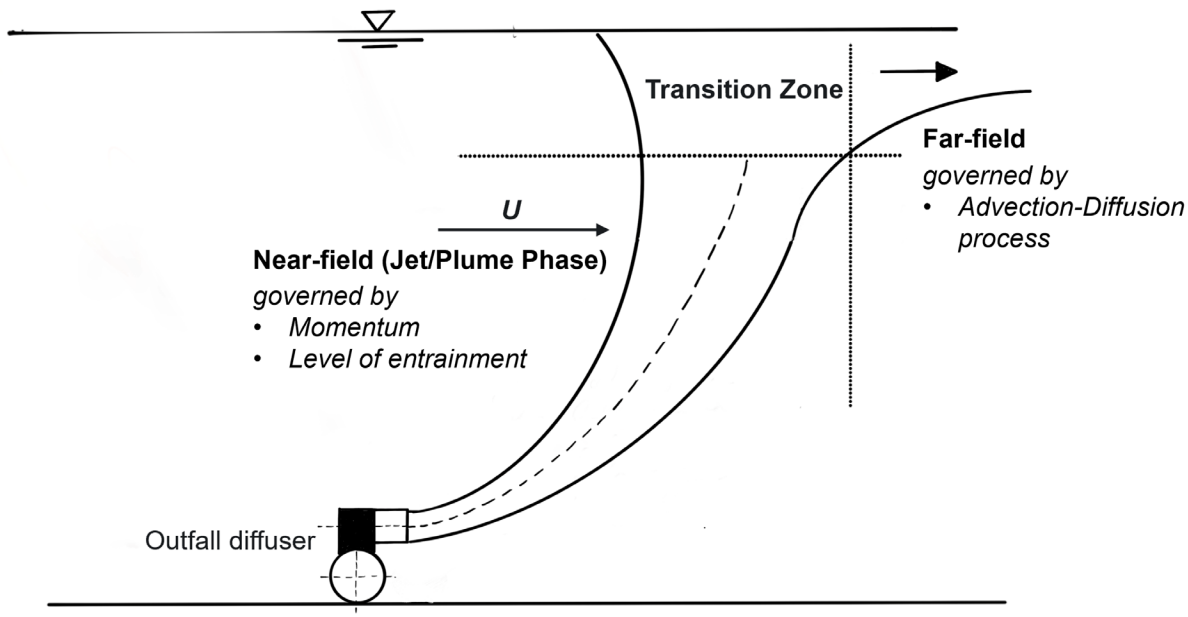


Figure 1 Schematical representation of the conceptual model for a typical effluent discharge.

Within a short distance from the ports, the flow entrains fluid and transitions from a jet to a plume. The buoyancy effects take over causing the plume to rise in the water column. As the plume ascends, it further entrains ambient water, diluting it and decreasing the plume buoyancy. When the buoyant plume is in a stratified water column, it stabilizes at a depth where its density approaches that of the surrounding water (the neutral buoyancy depth), trapping the plume below the water surface (also referred to as the trapping depth). In unstratified conditions, the plume often reaches the water's surface without being trapped. This region from the diffuser port to the stabilized wastefield is referred to as the zone of initial dilution (ZID) in secondary treatment regulations, or the region of rapid initial mixing in the scientific literature (Baumgartner et al., 1994; Roberts, 1990). For well-designed outfalls, the jet mixing is highly energetic near the outfall, resulting in rapid mixing and reduction in pollutant concentrations within the plume. The completion of the initial dilution phase, including jet and buoyancy effects, is typically constrained to a spatial scale of 10–1000 meters (m) and occurs over time scales of 1-10 minutes. After

the initial dilution is complete, the effluent is spread by ambient currents and diffusion by natural turbulence. The farfield mixing phase is governed by advection-diffusion and occurs over a much larger spatial scale of 100–10,000 m and time scales of 1-20 hours (Roberts, 1990).

2.2 Model Architecture

PLUMES2.0 follows the Visual Plumes approach to capture the nearfield plume characteristics while providing the option to continue the computations to farfield transport within a common computational framework. To facilitate this, the initial dilution component of PLUMES2.0 uses the Lagrangian Control Volume (LCV) method, as in the UM3 model (Baumgartner et al., 1994), including the entrainment and integrated features of plume merging. The farfield computations are conducted using the Brooks (1968) principles.

The architecture of PLUMES2.0 is also based on the mathematical and numerical approaches that were implemented in the UM3 model in Pascal code. In PLUMES2.0, each phase of the conceptual model was developed independently in Fortran 90 and includes the transfer of data from one phase to the next phase. Figure 2 shows a high-level representation of model design with data flow between different phases and processes. The model requires input related to (a) discharge characteristics such as diffuser layout, port orientation, diameter, flow rates, and (b) receiving water characteristics such as ambient stratification (temperature and salinity) and current velocity profile data. The jet/plume phase is numerically simulated using the LCV method. Upon the completion of nearfield computations, major plume parameters (i.e., plume diameter and dilutions) are revised/adjusted to match the wastefield dimensions (total width) during the transition stage prior to initiation of farfield calculations.

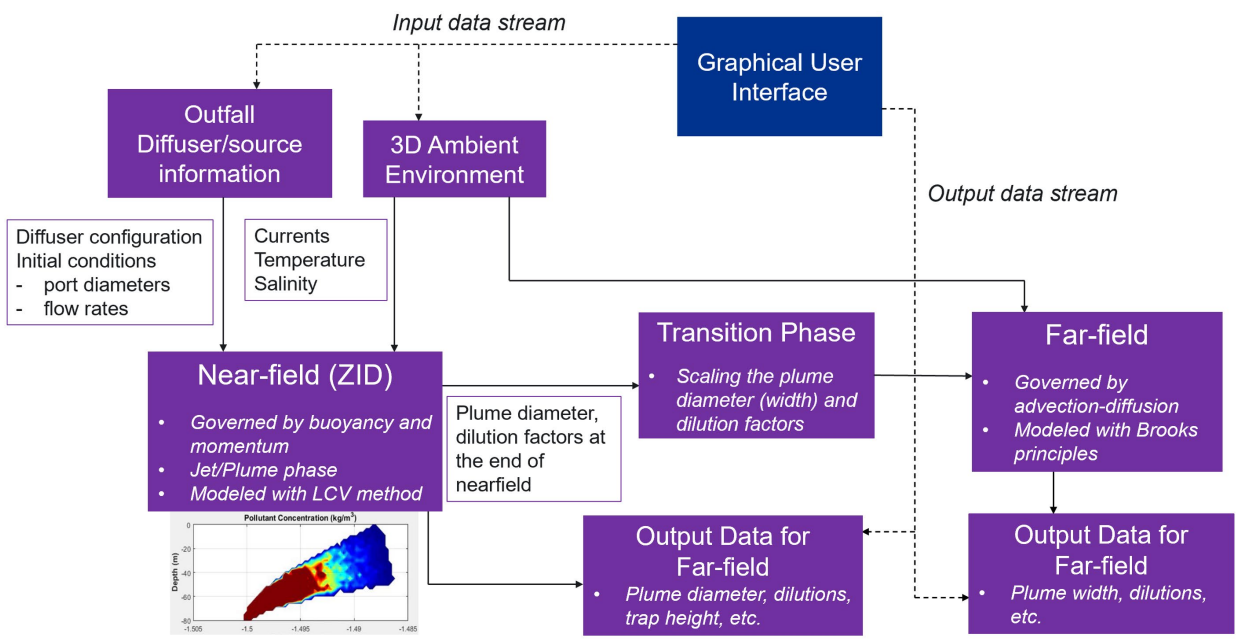


Figure 2: Schematic representation of the model architecture.

PLUMES2.0 was developed using Fortran 90 standards. Building and testing were conducted using Intel Fortran compilers. For the graphical user interface (GUI) development, several options were explored. Typical graphic libraries, application programming interfaces (APIs), and other tools are based

on C++, Python, and Java. Using such tools for GUI development creates coupling challenges with Fortran. To avoid the complexities and incompatibilities associated with coupling multiple programing languages, a Fortran 90 based GUI toolset was selected for the PLUMES2.0 GUI development. The commercially distributed third-party application – *Winteracter* (https://www.winteracter.com/) provided Fortran-based GUI libraries and development toolset for this effort.

2.3 Model Derivation

2.3.1 Near-Field Dilution

The plume behavior in the nearfield is simulated using the LCV method, adopting the approach that has been used previously in models such as UM3 and JETLAG (Baumgartner et al., 1994; Lee and Cheung, 1990). In the LCV method, the physical properties (i.e., velocities, concentration, salinity, etc.) of an LCV over a cross-section are assumed to be distributed uniformly using a Top-Hat profile structure. In other words, all properties at a specific plume cross-section are uniformly distributed and drop sharply to ambient values outside of the plume boundary. Figure 3 shows a schematic representation of selected LCVs of the plume, and the numerical integration of all LCVs produces the expected plume structure for the nearfield. The kinematic equations of the plume dynamics are derived by applying basic governing equations to each LCV of the plume. The continuity equation (Equation 2) describes the change in liquid mass in the LCV (dm) during a small-time increment (dt) is equal to the net ambient liquid entrainment. Total ambient entrainment is computed as the summation of forced entrainment and Taylor-induced entrainment (shear entrainment).

$$\frac{dm}{dt} = -\rho_a \boldsymbol{A_p}.\boldsymbol{U_a} + \rho_a A_T \beta_T \tag{2}$$

In Eq. 2, ρ_a is the density of the ambient liquid. $\boldsymbol{A_p}$ is the projected area vector for forced entrainment computation while $\boldsymbol{U_a}$ is the ambient velocity vector (vector variables indicated in bold). A_T is the area of the LCV in contact with ambient fluid for Taylor entrainment and wraps completely around the element is not expressed as a vector and computed as an area of a cylindrical element assuming an infinitesimal thickness of Lagrangian element (Baumgartner et al., 1994). β_T is the Taylor aspiration velocity, which can be defined as $\beta_T = \alpha|\boldsymbol{U_j}|$, where α is the Taylor entrainment coefficient and $\boldsymbol{U_j}$ is the average plume velocity of the LCV. $\boldsymbol{A_p}$ lies in a vertical plane containing the velocity vector and points upstream out of the element. $\boldsymbol{A_p}$ and $\boldsymbol{U_j}$ point in opposite directions so that their dot product is negative. To estimate the projected area, it is necessary to express mathematically how the length of the element changes in response to changes in other plume properties. Further details on the mathematical estimation of A_p can be found in Frick (1984) and Frick et al. (1995).

Eq. 3 represents the change of momentum in an LCV due to the momentum passed by the entrained ambient mass and the momentum induced by the buoyancy force acting on the LCV.

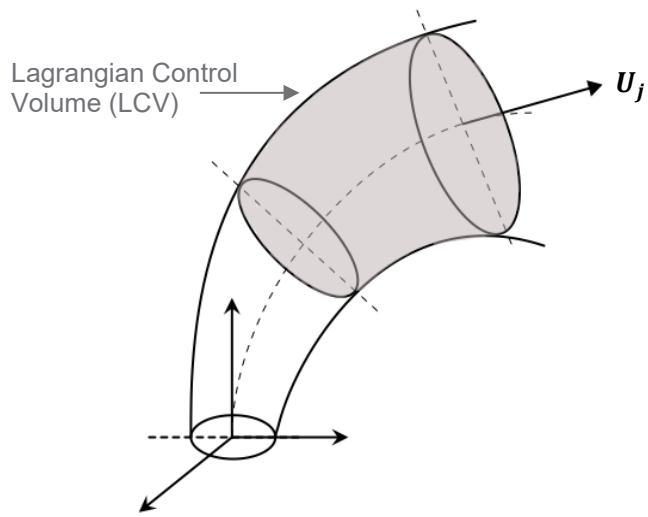


Figure 3: Lagrangian Control Volume representation (Premathilake and Khangaonkar, 2019).

Because the physical properties at the outer surface of the LCV are assumed to match the properties of ambient fluid, the drag force acting on the LCV is assumed to be zero, which is consistent with the approach of Baumgartner et al. (1994).

$$\frac{d(m\boldsymbol{U_j})}{dt} = \boldsymbol{U_a}\frac{dm}{dt} - m\frac{(\rho_a - \rho_j)}{\rho_j}\boldsymbol{g} \tag{3}$$

In Equation 3, g is the gravitational vector and ρ_j is the plume density of the LCV, which is a function of plume temperature and salinity. The plume temperature can be determined by applying the conservation of energy equation considering the heat exchange between the LCV and the ambient fluid. A simplified version of the energy equation has been used to compute the plume temperature in the dynamic phase of the plume, which is given by Equation 4,

$$\frac{d(mT_j)}{dt} = T_{\boldsymbol{a}}\frac{dm}{dt} \tag{4}$$

where, T_j and $T_{\boldsymbol{a}}$ denote the average plume temperature and temperature of ambient liquid, respectively. Eq. 4 was derived by assuming temporally constant specific heat at constant pressure, which is consistent with the approach followed in UM3 model formulation. Similarly, conservation of salinity is shown in Eq. 5, in which S_j and $S_{\boldsymbol{a}}$ are the average salinity of the LCV and ambient salinity, respectively.

$$\frac{d(mS_j)}{dt} = S_{\boldsymbol{a}}\frac{dm}{dt} \tag{5}$$

Both ambient and plume densities are computed from the equation of state for the sea water density (Sigma-t function) (Fofonoff, 1985). Numerical integration of the equations from Eq. 2 to Eq. 5, generates the spatial and temporal variation of the buoyant jet/plume properties.

To enhance rapid mixing and dilution of the effluent within the mixing zone, rather than releasing the effluent through an open-ended pipe, many outfall pipes include a diffuser section. The diffuser section of a typical ocean outfall is usually the most seaward section. The outfall pipe flow is blocked off with an end-flange, and the effluent is released through a series of ports. The ports may be simple holes directly

on the outfall pipe, or they may be designed with riser pipes normal to the diffuser axis. The ports may be fitted with nozzles with a port diameter that is relatively small and oriented at specific vertical angles, allowing the effluent to exit the outfall as a strong jet resulting in rapid entrainment and mixing. When the effluent is released from multiple ports, the individual plumes often merge with each other as the plumes rise in the water column, thereby affecting the individual plume dynamics. A schematic of a typical effluent plume from a multiport diffuser with plume merging is shown in Figure 4. Specifically, the merging processes affect the entrainment mechanism significantly as the individual plume area is reduced. This also results in a loss of dilution efficiency.

The merging of plumes causes a reduction in the effective plume area due to overlapping plume sections. The reduction in plume area reduces the overall entrainment causing changes to plume dynamics. Implementation of plume merging processes requires specific factors in the computation of the effective entrainment area. Figure 4 shows the reduction of plume areas in the overlapping plume sections. The mathematical formulation of UM3 introduced a geometry-based correction to calculate the entrainment area of merged plumes (Baumgartner et al., 1994). The same approach is adopted in the mathematical model of PLUMES2.0.

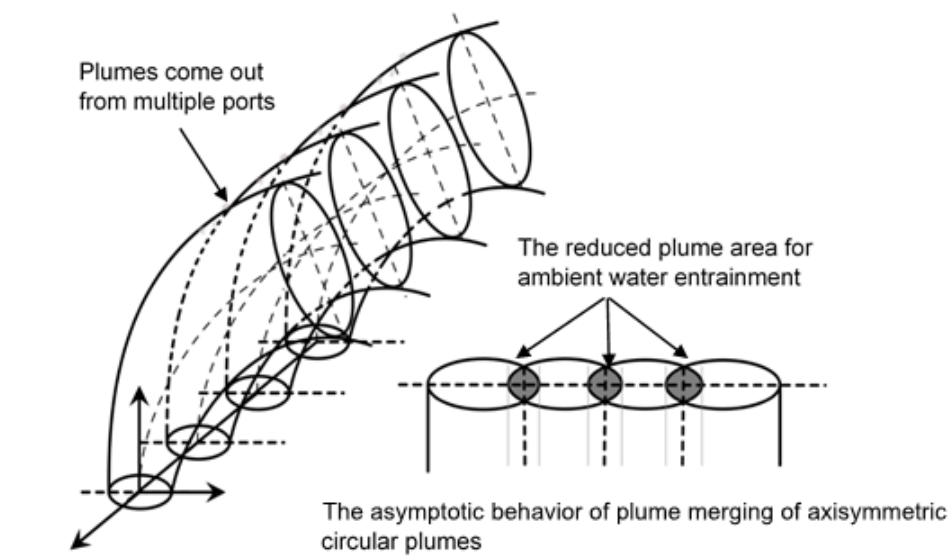


Figure 4: Typical merging model for vertically released effluent discharges.

The model development presented above is based on average motion of the plume element with properties averaged over the element. The plume trajectory is traced by the center-of-mass of the plume element. The plume element expands with time as it moves away from the source, affected by buoyancy and entrainment of ambient water, with widely varying properties in between the element boundaries. The concentration of the effluent mass averaged over the Lagrangian element (C_{ave}) is computed by the model in each step based on volume of water entrained in the element. The assumption is that the effluent mass in the Lagrangian element at each time step remains constant. Of importance is the calculation of difference in concentration between the plume and the ambient (C_{ave}-C_a), where C_a is the ambient concentration. Dilution in the plume relative to initial effluent concentration at the end-of-the pipe C_e is

given by $D = \frac{(C_e - C_a)}{(C_{ave} - C_a)}$, as in Equation 1 after rearranging the terms. Here, C_{ave} computed by the model in each model step replaces C_f at the end of initial dilution process (in Equation 1).

In the model, the concentrations are assumed to be distributed over the cross section of the plume element following the 3/2 power profile (Kannberg and Davis, 1976), which closely matches a Gaussian profile but is constrained to the plume geometry. The 3/2 power profile is expressed by the following.

$$\Phi = \left[1 - \left(\frac{r}{b}\right)^{\frac{3}{2}}\right]^2 \tag{6}$$

where, as described in Baumgartner et al. (1994), Φ is an instantaneous scaling factor relating difference between the plume and the ambient of any appropriate property, such as the concentration of some pollutant or velocity, b is the plume radius, and r is the distance from the center of the plume to the point within the plume at which Φ is measured. In other words, $C(r) = C_{max} \cdot \Phi$. This distribution ensures maximum concentration is at r = 0, at the plume element centerline and approaches 0 for r = b at the radial plume boundary.

The average concentration C_{ave} provided by the model may also be expressed as flux-averaged concentration.

$$C_{ave} = \frac{\int C \cdot v \cdot dA}{\int v \cdot dA} \tag{7}$$

where C and v are the instantaneous concentration and velocity in the plume element at a radial location r distance from the centerline, A is the cross-sectional area, and dA is the corresponding infinitesimal area. For large dilutions and currents, the velocity may be approximated to follow a top-hat distribution and assumed constant. This simplification along with 3/2 profile for concentrations (substituting C with $C_{max} \cdot \Phi$) can be used to derive the relationship $\frac{C_{max}}{C_{ave}} = 3.89$ for round plumes and 2.22 for fully merged line plumes. However, as described in Baumgartner et al. (1994), the ratios can vary. In much of the plume, the peak-to-mean ratios are considerably smaller than these limiting values, approaching 1.0 at the source. Therefore, the centerline concentration prediction is approximate and occasionally deviates from the expected trend when vertically varying background pollutant concentrations are present. The dilution value D computed by the model by default is the flux-averaged dilution, based on flux-averaged concentration C_{ave}. The centerline dilution (an output provided by the model) corresponds to C_{max}.

The termination of the plume dynamic phase is decided by four benchmarks based on the plume properties. The first criterion, which decides the termination of the nearfield mixing, is the stage in which the plume density is equal to the ambient density. This also can be defined as the plume-trapping stage, and the depth at which the plume reaches neutral buoyancy, designated as the trapping depth. The second criterion for terminating the nearfield mixing is when the plume vertical velocity becomes reversed, causing the plume that has overshot the trapping depth to fall back. Once the plume reaches this stage, the plume structure collapses, and subsequent effluent transport continues as an advection-diffusion process. Other criteria for the termination of jet/plume behavior of the effluent plume include instances such as when the plume encounters boundaries, including the water surface, the shoreline, or the seabed.

2.3.2 Far-Field Dilution

Once the momentum-driven plume reaches the terminal criterion of nearfield dilution, the plume structure is no longer sustainable and is dispersed as a passive effluent field by the ambient currents. Here, the effluent (which exited with an initial end-of-pipe concentration of C_e) is already partially mixed in the ambient environment after completion of initial dilution process (dilution ratio D) with a resulting wastefield concentration of C_o. Further mixing and dilution occurs with time as the plume travels away from the zone of initial dilution, through natural turbulent diffusion that slowly reduces the wastefield concentration from C_o to $C(x,y,z)$, asymptotically reducing towards the background concentration. Farfield dilution factor FF may then be defined as $FF=C_o/C(x,y,z)$. Final effluent dilution at specified farfield location is then given by $D_{farfield} = D \cdot FF$. This determination of final farfield dilution factor requires calculation of $C(x,y,z)$. The conventional approach is to solve for $C(x,y,z)$ using the 3D advection-diffusion equation in the form shown below.

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(\epsilon_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\epsilon_z \frac{\partial C}{\partial z}\right) \tag{8}$$

Here, the effluent field concentration (in kg/m^3) is denoted by C, and $u, v,$ and w are ambient velocities (m/s) in x, y, and z directions, respectively. ε_x, ε_y, and ε_z are the corresponding eddy diffusivities (m^2/s) in x, y, and z directions. As in Visual Plumes, the PLUMES2.0 uses Brooks principles (Brooks, 1960) to compute the farfield spreading of the wastefield and associated dilution over time and Brooks principles are based on a simplified one-dimensional and steady-state version of the Equation 8, as shown below:

$$u\frac{\partial C}{\partial x} = \frac{\partial}{\partial y}\left(\epsilon_y \frac{\partial C}{\partial y}\right) + kC \tag{9}$$

where k is the transformation rate of the effluent which may be growth rate or decay rate depending on the nature of non-conservative constituent. For typical Brooks farfield applications, k value is set to zero. The primary premise for Brooks principles is that the wastefield grows laterally with distance (Figure 5). The lateral growth is caused by turbulent mixing, represented by the lateral diffusion coefficient (ϵ_y). Brooks laws were derived by solving Equation 9 analytically via length scaled relationships for ϵ_y.

A summary of Brooks principles is shown in Table 2 showing the growth of eddy diffusivity and plume width as a function of distance. Brooks provided three case types for lateral mixing giving consideration for environmental conditions. Case 1 represents narrow river or channel where eddy diffusivity may be assumed to be constant. Case 2 represents estuarine conditions where eddy diffusivity may be expected to grow linearly with distance from the outfall. Case 3 represents open ocean conditions where eddy diffusivity was derived by Brooks to apply the 4/3rd power law relationship to the plume width.

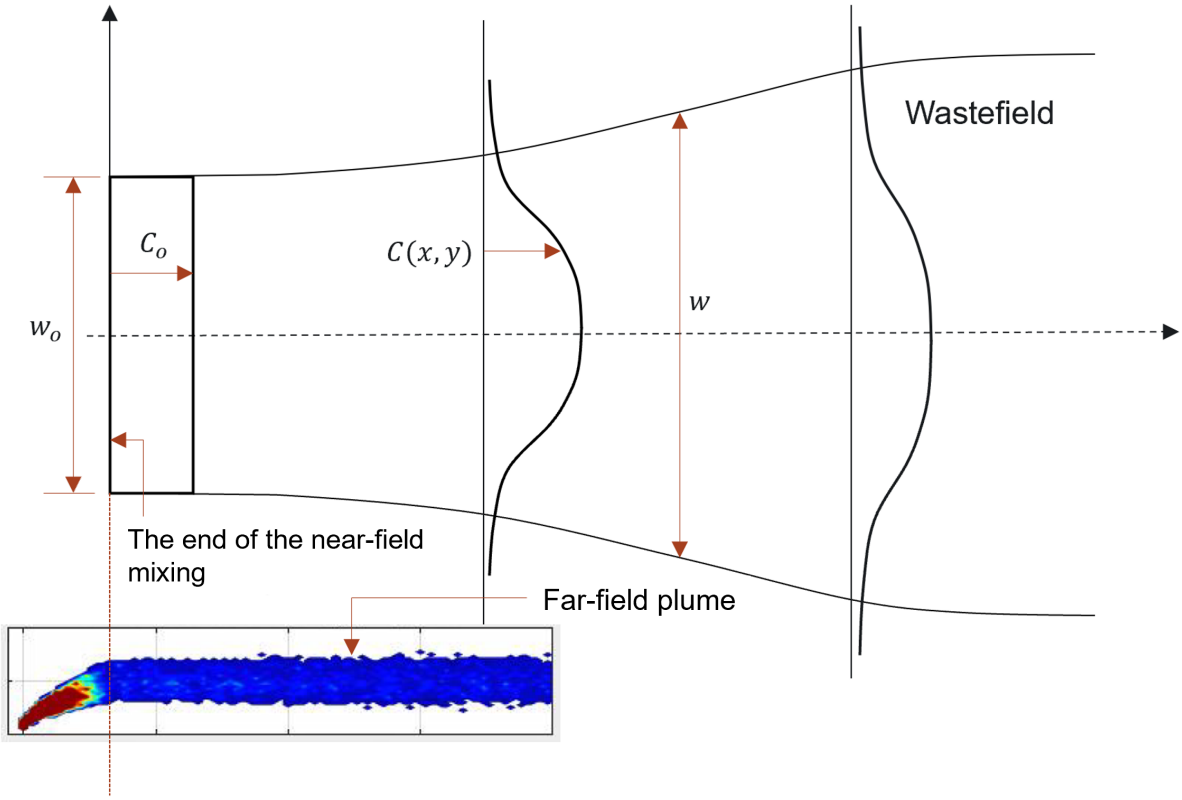


Figure 5: Schematic representation of a typical far-field plume growth under steady conditions. The inset with color contours represents a vertical cross section that shows the initial dilution phase as well as the far-field transport. (Note: vertical spreading is assumed to be negligible in Brooks' far-field model calculations)

Table 1: Variation of Width of Wastefield with Distance

Case 1	Constant ϵ	$\frac{\epsilon}{\epsilon_o} = 1$	$\frac{w}{w_o} = \left(1 + 2\beta\frac{x}{w_o}\right)^{1/2}$	(10)
Case 2	Linear increase in ϵ	$\frac{\epsilon}{\epsilon_o} = \frac{w}{w_o}$	$\frac{w}{w_o} = \left(1 + 2\beta\frac{x}{w_o}\right)$	(11)
Case 3	4/3-Law	$\frac{\epsilon}{\epsilon_o} = \left(\frac{w}{w_o}\right)^{4/3}$	$\frac{w}{w_o} = \left(1 + \frac{2}{3}\beta\frac{x}{w_o}\right)^{3/2}$	(12)

w_o =initial width of sewage field ($w/w_o = 1$ at $x = 0$), Note, the origin or x = 0 in Brooks' calculations represents the location of the wastefield after initial dilution is complete and is different from the origin for initial dilution calculations at the outfall port. w = width at a distance x (x = u·t) from the start of far-field calculations. ϵ is the eddy diffusivity at a distance x, and ϵ_o is the initial eddy diffusivity.

$$\beta = \frac{12\epsilon_o}{u \cdot w_0} \text{ (dimensionless)} \quad (13)$$

The far-field dimensions of the wastefield are computed using the above rules and corresponding dilutions at the center of wastefield (i.e., lowest dilutions or maximum concentration).

Table 2 provides the resulting equations used to calculate constituent concentration or far-field dilution factor FF=*(C_0/C)* in the wastefield for the three cases, and as defined previously, $D_{farfield} = D \cdot FF$.

Table 2: The analytically-derived concentrations at the center of the wastefield (Brooks, 1960)

Case 1	$\frac{\epsilon}{\epsilon_o} = 1$	$C(x) = C_o e^{-kt} \mathrm{erf} \sqrt{\frac{3}{4\beta x / w_o}}$	(14)
Case 2	$\frac{\epsilon}{\epsilon_o} = \frac{w}{w_o}$	$C(x) = C_o e^{-kt} \mathrm{erf} \sqrt{\frac{3/2}{\left(1+\beta\frac{x}{w_o}\right)^2 - 1}}$	(15)
Case 3	$\frac{\epsilon}{\epsilon_o} = \left(\frac{w}{w_o}\right)^{4/3}$	$C(x) = C_o e^{-kt} \mathrm{erf} \sqrt{\frac{3/2}{\left(1+\frac{2}{3}\beta\frac{x}{w_o}\right)^3 - 1}}$	(16)

3.0 Carbonate chemistry and equilibrium kinetics

3.1 Introduction

The marine carbonate system is a natural buffering system that regulates the pH of seawater through a series of chemical reactions involving carbon dioxide (CO_2), water (H_2O), and bicarbonate (HCO_3^-) and carbonate (CO_3^{2-}) ions. When CO_2 dissolves in seawater, it forms carbonic acid (H_2CO_3), which then releases hydrogen ions (H^+) and HCO_3^- ions, causing a slight drop in pH (increase in acidity). This natural balance is a critical component of ocean biogeochemistry, that influences biological productivity and marine water quality. The natural balance can be affected by wastewater discharges which could be acidic or basic in their ionic strength.

Seawater pH serves as a sensitive indicator of acid–base conditions, and even small deviations can significantly influence biological and chemical processes, including nutrient cycling, and the physiology of calcifying organisms. Dissolved inorganic carbon (DIC), primarily comprising of aqueous CO_2, HCO_3^-, CO_3^{2-} ions, represents the dominant form of inorganic carbon in seawater which is central to biological productivity. Total alkalinity (TA) defined as the excess of proton acceptors over proton donors, represents the seawater buffering capacity and helps stabilize pH under variable biogeochemical and anthropogenic stressors. Effluents from desalination plants, industrial processes, or municipal wastewater treatment facilities can introduce substantial quantities of dissolved inorganic species, nutrients, and alkalinity into receiving marine waters through outfalls. Most states in the US have water quality standards for pH that wastewater discharges must comply with. Carbonate chemistry calculations in combination with effluent plume dilution and mixing are needed to estimate pH levels at the regulatory mixing zones.

In recent years, there has been an added interest in modeling the effects of high-alkalinity effluents. Ocean alkalinity enhancement (OAE) approach is an emerging technology that has the potential to accelerate marine CO_2 removal while providing the added benefit of local ocean acidity reduction (NASEM 2022). However, high alkalinity discharges also tend to be high in pH and have the potential impact marine biota. Also, the effectiveness of this treatment depends strongly on the magnitude of the discharge, its composition (pH, TA, DIC) and the dilution and mixing of the discharge with the ambient. If high alkalinity effluent is introduced without adequate dilution, the aragonite saturation state (Ω_{arag}) may exceed threshold levels (≈ 5, Moras et al. 2019) and result in loss of DIC through runaway precipitation of carbonate, resulting in loss in efficiency of the high alkalinity enhancement. Therefore, in addition to computing pH, TA, and DIC levels as part of Mixing Zone compliance analysis, there is also interest in computing the equilibrium kinetics from an engineering feasibility perspective for high alkalinity releases.

To support the regulatory and user community needs, PLUMES2.0 was modified to include carbonate chemistry calculations that simulate the pH-TA-DIC equilibrium while accounting for dilution and mixing along the effluent plume trajectory.

3.2 PLUMES2.0 Carbonate Chemistry Formulation

Carbonate chemistry calculations in PLUMES2.0 were incorporated under the assumption that equilibrium of pH-TA-DIC inside a plume element (LCV) occurs instantaneously along with ambient mixing. The TA and DIC are scalar constituents defined in each plume element, which undergo entrainment induced ambient mixing as plume progresses (Eqs. 17 and 18). The impact of biological

activity on TA and DIC within the plume is neglected as relatively large changes to TA and DIC are caused by rapid ambient mixing over short timescale of minutes.

$$\frac{d\left(m\,(TA)_j\right)}{dt} = (TA)_a \frac{dm}{dt} \tag{17}$$

$$\frac{d\left(m\,(DIC)_j\right)}{dt} = (DIC)_a \frac{dm}{dt} \tag{18}$$

In Eq. 17, $(TA)_j$ and $(TA)_a$ are the average total alkalinity of the plume/jet and the ambient water respectively. Similarly, in Eq. 18, $(DIC)_j$ and $(DIC)_a$ are the average dissolved inorganic carbon of the plume/jet and the ambient water. The pH of the plume ($(pH)_j$) is computed based on the $(TA)_j$ and $(DIC)_j$ concentrations using CO2SYS procedures. CO2SYS is a software package used by oceanographers to calculate the properties of the carbon dioxide system in seawater and freshwater (Lewis and Wallace 1998). As part of this effort, the CO2SYS routines were incorporated directly into PLUMES2.0 to calculate the K_1, K_2 and K_{so4} carbonic acid and sulfuric acid disassociation coefficients. The pH-TA-DIC balance computed by the PLUMES2.0 was then validated using the latest CO2SYS software version available in python as PYCO2SYS (Humphreys et al., 2022).

In addition to pH-TA-DIC equilibrium, aragonite (Ω_{arag}) and calcite (Ω_{calc}) saturation state calculations for the two forms of calcium carbonate were incorporated into PLUMES2.0. These outputs in the near-field zone of initial dilution allow assessment of the impacts and help estimate the potential for calcification and runaway precipitation for high alkalinity releases. In general, $\Omega > 1$ indicates supersaturation, where seawater is rich enough in carbonate ions for aragonite or calcite to readily form and precipitate. This condition is favorable for marine organisms like corals and shellfish that use aragonite to build their shells and skeletons, and it suggests a lower risk of dissolution compared to undersaturated and acidic conditions with $\Omega < 1$. Also, Ω values must remain below the threshold of 5 to avoid runaway precipitation in high alkalinity effluent releases (Moras et al. 2022).

The saturation states are computed based on solubility ratios as shown in Eqs. 19 and 20 below.

$$\Omega_{\text{arag}} = \frac{[CO_3^{2-}][Ca^{2+}]}{K_{\text{sp,arag}}} \tag{19}$$

$$\Omega_{\text{calc}} = \frac{[CO_3^{2-}][Ca^{2+}]}{K_{\text{sp,calc}}} \tag{20}$$

$K_{\text{sp,arag}}$ and $K_{\text{sp,calc}}$ are the solubility coefficients which are computed based on temperature (T) and salinity (S) per Millero (1995). $[Ca^{2+}]$ - calcium ion concentration is calculated using a salinity-based relation (Murata et al., 2015) $[Ca^{2+}] = 0.01028 \times \frac{S}{35}$. $[CO_3^{2-}]$ - carbonate ion concentration calculated is based on K_1, K_2 and $[H^+]$ (Eq. 21).

$$[CO_3^{2-}] = \frac{(DIC)K_1K_2}{[H^+]^2 + K_1[H^+] + K_1K_2} \tag{21}$$

PLUMES2.0 also directly computes the potential precipitation rates for aragonite and calcite to evaluate the immediate risk of high alkalinity releases. The precipitation rates are estimated based on an empirical reaction order (N) per Zhong and Mucci (1989). The precipitation model is shown as in Eq. 22.

$$\log R = N \log\left(\Omega_{\frac{\text{calc}}{\text{arag}}} - 1\right) + \log K \tag{22}$$

In eq. 22, R is the precipitation rate (μmol/hr) and K is the rate constant. Both N and K are determined based on the experimental data. While PLUMES2.0 uses default values for N and K from Zhong and Mucci (1989) for defined salinity ranges, it offers the flexibility for users to change these parameters derived for recent experimental/laboratory data. Also, it should be noted that PLUMES2.0 only calculates the potential precipitation rate explicitly for each plume element and does not dynamically simulate the conservation of precipitated mass.

4.0 Biochemical oxygen decay and dissolved oxygen

4.1 Introduction

Municipal wastewater outfalls typically discharge effluent with dissolved oxygen (DO) levels considerably lower than the ambient DO and often below applicable water quality standards. DO levels in municipal wastewater discharges may range from 2 to 4 mg/L, with some plants achieving higher levels with advanced treatment. Raw wastewater has very low DO (often below 1 mg/L). In addition, municipal and some industrial wastewaters are high in biochemical oxygen demand (BOD). Biochemical oxygen demand is determined through laboratory incubation of the water sample for five days at 20°C and measuring the change in dissolved oxygen (BOD_5). Natural pristine waters have BOD_5 levels < 1 mg/L while typical municipal wastewater with secondary treatment have BOD_5 < 30 mg/L by design. As a result, improved DO levels following mixing with high DO in the ambient or receiving waters may drop further as the plume travels away, and the maximum DO impact may occur well beyond the mixing zone and long times (days).

As part of the NPDES permit compliance assessments, regulators and permittees are often faced with the question – "What is the DO concentration at the mixing zone following initial dilution?" and "What is the maximum DO depletion resulting from the wastewater discharge" in the study area. While this may be addressed through a detailed study using site specific complex 2-D or 3-D biogeochemical models, it is often beyond the scope where screening level conservative estimates may suffice. To address this, US EPA developed a simplified procedure to estimate far-field DO impacts for marine outfalls based on Brooks (1960) far-field dilution (see Amended Section 301(h) Technical Support Document. EPA 842-B94 -007, 1994). It is a two-step procedure involving a combination Initial Dilution Model, the Brooks far-field model, and calculation of DO depletion through biochemical oxygen demand including dilution effects.

To support the regulatory and the user community needs, PLUMES2.0 was modified to include a simplified BOD-DO model which simulates the depletion of DO due to BOD, including DO minima in the far-field and subsequent recovery over time and distance through entrainment of ambient DO rich waters.

4.2 DO/BOD model formulation

Model formulation as described in US EPA (1994) was incorporated here. The effect of BOD on DO during the initial dilution process is considered negligible. However, some effluents contain substances that are easily reduced when entering marine/saline environments. This is known as immediate DO demand (IDOD) which may at times be significant and must be accounted for.

As a first step, DO concentration at the end of initial dilution process must be determined before farfield calculation accounting for BOD impact can begin. Final DO at the termination of initial dilution process is given by the following equation.

$$DO_f = \left(\frac{DO_e - IDOD - DO_a}{D}\right) + DO_a \tag{23}$$

where DO_f = Final DO concentration (mg/L) of the effluent after initial dilution and mixing with the ambient water,

DO_e = Effluent DO concentration (mg/L) in the discharge or end-of-pipe concentration,
$IDOD$ = Immediate DO demand, mg/L
DO_a = Ambient or receiving water concentration (mg/L), typically upstream from the discharge, and
D = the nearfield dilution ratio (flux-averaged initial dilution)

Typical IDOD values vary from 0 to 10 mg/L depending on the level of treatment (raw to primary). For municipal effluent with advanced primary treatment (and higher) IDOD is typically < 1 mg/L (US EPA 1994) and likely lower or negligible for effluents with secondary treatment.

BOD consists of two components, the carbonaceous BOD and nitrogenous BOD measured using the standard 5-day test, denoted as $cBOD_5$ (mg/L) and $nBOD_5$ (mg/L). Although 5-day BOD represents most of the demand, it is lower than the ultimate demand reached asymptotically at time = ∞. Ultimate carbonaceous and nitrogenous BOD are given by the following equations.

$$cBOD_L = \frac{cBOD_5}{(1 - e^{-k_c t})} \tag{24}$$

where, k_c = $cBOD_L$ decay rate at temperature T°C, d^{-1}
t = 5, the elapsed time in days
$cBOD_L$ = ultimate carbonaceous BOD, mg/L

$$nBOD_L = \frac{nBOD_5}{(1 - e^{-k_n t})} \tag{25}$$

where, k_n = $nBOD_L$ decay rate at temperature T°C, d^{-1}
t = 5, the elapsed time in days
$nBOD_L$ = ultimate nitrogenous BOD, mg/L

In the absence of site specific data, the values 0.23 d^{-1} and 0.1 d^{-1} are suggested as defaults for k_c and k_n respectively, but readers are referred to guidance from US EPA (1985) and US EPA (1994) to make their own informed decisions on selection of suitable BOD decay rates. This includes temperature correction for decay rates in the field relative to 20°C laboratory temperatures. The correction term has the following form.

$$k_c(T) = k_c(20) \cdot \theta_c^{(T-20)} \tag{26}$$

and

$$k_n(T) = k_n(20) \cdot \theta_n^{(T-20)} \tag{27}$$

where T (°C) is the site specific ambient temperature and θ_c and θ_n are temperature correction factors for nitrogenous and carbonaceous BOD decay rates. Guidance provided in US EPA (1985) and US EPA (1994) suggests that a θ_c = 1.047 and θ_n = 1.08 may be used as defaults over most temperature ranges buts values could be higher for temperatures below 10°C.

Following initial dilution, as the wastefield plume is carried away, the diluted BOD begins to draw the DO levels down over timescales of hours or days. The DO depletion rate is proportional to the ultimate BOD concentration(s) in the wastefield after initial dilution, above the ambient defined as follows.

$$L_{fc} = \frac{(cBOD_{Le} - cBOD_{La})}{D} \tag{28}$$

and

$$L_{fn} = \frac{(nBOD_{Le} - nBOD_{La})}{D} \tag{29}$$

where, $cBOD_{Le}$ = ultimate carbonaceous BOD in the effluent, mg/L
$nBOD_{Le}$ = ultimate nitrogenous BOD in the effluent, mg/L
$cBOD_{La}$ = ultimate carbonaceous BOD in the ambient, mg/L
$nBOD_{La}$ = ultimate nitrogenous BOD the ambient, mg/L
D = Nearfield dilution ratio (flux-averaged initial dilution)
L_{fc}= Ultimate cBOD concentration above ambient at the completion of initial dilution, mg/L
L_{fn}= Ultimate nBOD concentration above ambient at the completion of initial dilution, mg/L

Finally, DO as a function of travel after initial dilution - $DO(t)$, mg/L is given by the simplified DO depletion model based on Brooks (1960) far-field dilution calculations as follows.

$$DO(t) = DO_a + \frac{(DO_f - DO_a)}{FF} - \frac{L_{fc}}{FF}(1 - e^{-k_c t}) - \frac{L_{fn}}{FF}(1 - e^{-k_n t}) \tag{30}$$

where, FF is the far-field dilution factor given by the appropriate Brook's eqn. -14, 15, or 16 based on the type of lateral mixing selected.(constant, linear, or 4/3rd power law). DO_f is computed using eqn. 23.

5.0 PLUMES2.0 User Instructions

5.1 Download and installation

PLUMES2.0 software is distributed in the form of a self-extracting zip file that may be downloaded from the following locations.

U.S. EPA's Center for Exposure Assessment Modeling via the following link.
https://www.epa.gov/hydrowq/PLUMES2.0

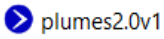
or

from the University of Washington SSMC GitHub site for the PLUMES2.0v1 update.
https://github.com/ssmc-uw/PLUMES2.0

Download the zip file "PLUMES2.0-main.zip" from the U.S. EPA site, or, from the GitHub site, download by clicking

the Code (green) button.

Copy the zip file from the download folder to your designated folder (e.g., C:\Users\useraccount\Desktop\) and extract the files using Windows explorer. The operating system requirements are Windows 10 or higher. The extracted folder, named \plumes2.0-main, contains additional subfolders (\icons, \images, and \Example_project), multiple utility files, and the plumes2.0 or plumes2.0v1executable if downloaded from the SSMC GitHub site.

Launch the application by double clicking the icon. 

Windows defender may require your approval to run the application as it may not be recognized by Windows. [click "more information" prompt and select "run anyway" option.] Having an organizational IT-Admin assisted install may be required if the user does not have administrative privileges. We recommend the option to right click the icon and select "pin to task bar" for convenient future access.

5.2 PLUMES2.0 User Interface

The PLUMES2.0 user interface was set up to mimic many features of the Visual Plumes software to allow seamless transition for the Visual Plumes community. Experienced users will recognize the diffuser, effluent, and ambient tabs for entering project-specific data. The "*Welcome*" screen or tab introduces PLUMES2.0, and additional information is also available under the "*About*" tab.

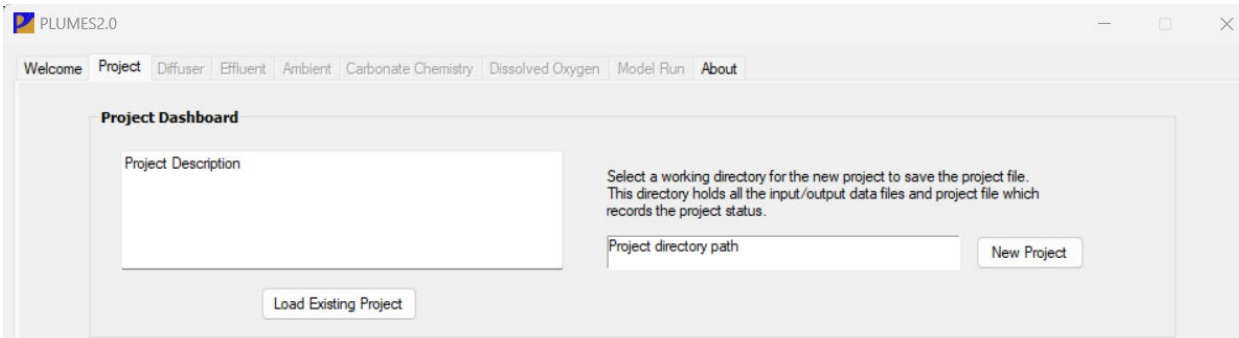
Click the "*Project*" tab or the icon to start using PLUMES2.0.

5.2.1 Project set up

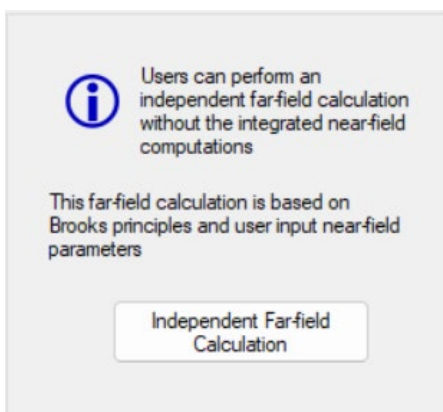
The *Project* tab screen provides step by step instructions on how to set up a new project scenario. The window under the project dashboard (Project Description) allows the user to enter project specific information and details. This could include the outfall name, project owner, project site location and serve as a project identifier. Immediately below is the *Load Existing Project* button. This allows the user to upload previously saved project configuration and data to continue prior work, or to run additional scenarios without having to re-enter the project and case-specific information.

For a new project, click the *New Project* button. It opens a Windows explorer style menu. Navigate to the directory where you would like to conduct model runs, right click in the selected directory to create a new project folder. Double click to enter the new project folder, provide a project file name and hit the

save button. The project data and configuration that will be entered in subsequent steps will be saved automatically under the project file name once the model run is executed. The saved project information may be reloaded if the user wishes to close the program and return to it later, thereby avoiding the need to re-enter the input data. Once the New Project is created, the tabs - *Diffuser*, *Effluent*, and *Ambient* for entering project specific data become available along with the *Model Run* tab to run the dilution calculations (see below).



Also provided on the *Project* page is an added feature or option *Independent Far-field Calculation* to allow stand-alone simulation of far-field transport of a wastefield using Brook's far-field transport algorithm. This allows the user to estimate far-field plume transport independent of the near-field dilution process (see Section 3.2.7).



5.2.2 Diffuser characteristics

Wastewater effluent is typically discharged to the surface waters through an outfall pipe. To increase jet-induced mixing and initial dilution, the outfall design often includes a diffuser section, located at the end of the outfall pipe. Rather than discharge directly through a pipe with a large diameter and low velocities, the effluent is released under pressure through multiple ports with small diameters, and therefore at higher (jet) velocities. This section of the outfall pipe with multiple ports arranged in a row is called the diffuser section. The strong mixing provided by the diffuser also helps trap the wastefield lower in the water column at the end of the buoyancy-induced mixing phase.

Outfall designs vary from the simplest configuration of an open-ended outfall pipe (single port) to complex multiport diffusers with ports at the end of risers arranged uniformly or in a fan or with alternating angles to maximize efficiency in settings with reversing tidal currents. The UM3 code is

designed for single-port or multiport diffusers with uniformly arranged ports. Diffuser configuration consists of the following parameters.

1. Port diameter : Diameter (assuming circular opening) or equivalent diameter, m
2. Port elevation : Distance from the seabed to port center, m
3. Vertical angle : Angle of port/discharge vector to horizontal plane, +tive counter-clockwise from x-axis
4. Horizontal angle : Angle of port/discharge vector to vertical plane, +tive counter-clockwise from x-axis
5. Number of ports : 1 = single port outfall, n = multiport diffuser with n ports
6. Port spacing : Distance between ports, m (or average spacing for irregular diffusers)
7. Port depth : Distance from water surface to the port centerline
8. X and Y coordinates : Diffuser location or the starting point for the plume calculations

Figure 6 provides a schematic representation of a submerged outfall and diffuser configuration defining the parameters for setting up a project run.

Click the *Diffuser* tab to see a simplified version of Figure 6 and a table where numeric values for the diffuser parameters may be entered. The user also has an option to load a previously saved diffuser configuration. Click the *Load* button to load "Diffuser_example.csv" file. This file is in the Example_project folder. Figure 7 shows that the example diffuser has 18 ports spaced 6.1 m apart. Each port is on a riser pipe with a port diameter of 0.076 m. Each port is angled up at 45° to the horizontal plane. The horizontal angle of the discharge vector is at a 30° angle to the x-axis which is also the direction of the ambient current. The diffuser location (X, Y) coordinate is specified using the centerline of the middle port or the mid-point of the diffuser section (the user may select any arbitrary location for the origin, and orientation of x-axis). Selecting an x-axis along the shoreline or along the current direction simplifies data entry. The port elevation is 0.31 m and port depth at the diffuser is 11 m. Check the case button to select this diffuser. The table may be populated with multiple diffuser designs but only the checked diffuser configuration is used in calculations. All inputs are saved to the project file automatically upon model run. But the user may wish to save the selected diffuser configuration for later re-use. Additional notes on diffuser configuration:

- Port depth plus port elevation equals water depth at the diffuser location. However, water depth away from the diffuser may be greater and may be entered via the *Ambient* tab. The ambient tab allows entry of water profiles at a representative ambient location which may be different from the diffuser site and deeper.
- The data entry by default for all parameters is in SI system of units, but the user may use the drop-down arrows on the unit cell in the respective column to switch to FPS system. Note that all model results are provided in the SI units only.
- The *Model Run* tab (described later in Section 3.2.5) has two additional characteristics related to the outfall/diffuser for user entry: diffuser contraction coefficient and distance to nearest shoreline.
- The port elevation may be set to zero. However, initial dilution will be terminated as the plume will immediately touch the bottom. The user will need to shut off "stop the plume at bottom hit" criterion on the *Model Run* tab.
- The model cannot be applied for surface discharges. Port depth cannot be zero. Similarly, port elevation cannot equal port depth.
- All ports must face the same direction.
- There is no limit on the number of ports, but it is assumed that the diffuser design provides sufficient exit velocity (densimetric Froude number, $Fr = U/\sqrt{gD(s-1)} > 1$) to prevent

salinity intrusion. Here, *U* and *D,* are port velocity and port diameter, respectively, and '*s'* is the ratio of ambient and effluent densities.

Note that the entered information is not saved until the model run is executed. The diffuser configuration may be saved using the *"Save"* button. Similarly, previously saved diffuser configuration may be loaded using the *"Load"* button.

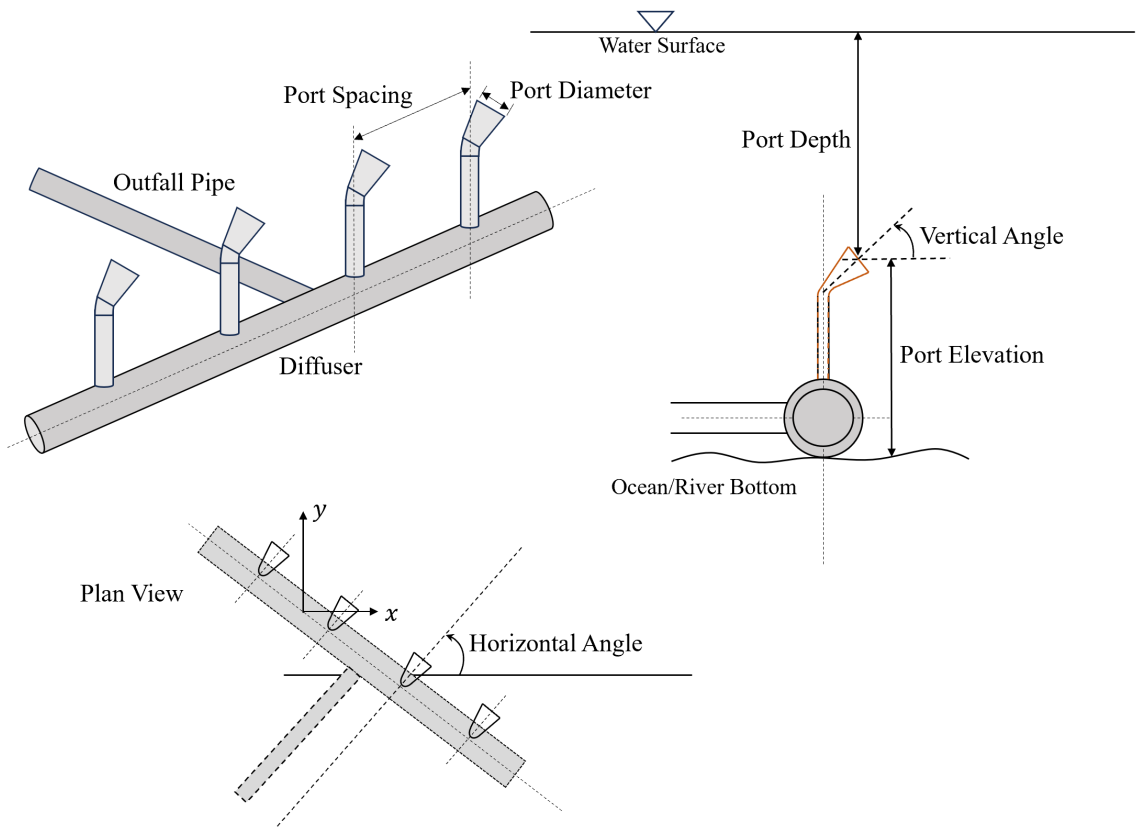
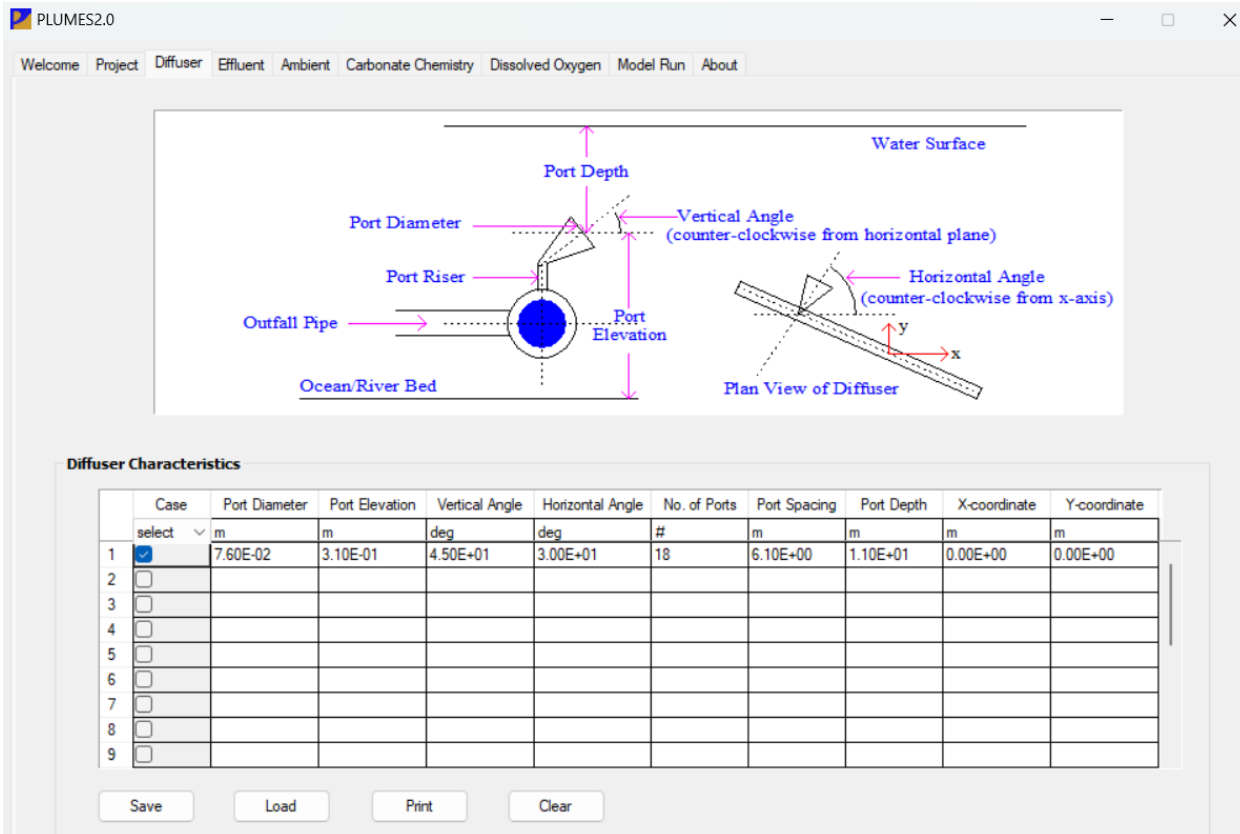


Figure 6: Schematic representation of outfall pipe and definition of diffuser parameters.



	Case	Port Diameter	Port Elevation	Vertical Angle	Horizontal Angle	No. of Ports	Port Spacing	Port Depth	X-coordinate	Y-coordinate
	select	m	m	deg	deg	#	m	m	m	m
1	☑	7.60E-02	3.10E-01	4.50E+01	3.00E+01	18	6.10E+00	1.10E+01	0.00E+00	0.00E+00
2	☐									
3	☐									
4	☐									
5	☐									
6	☐									
7	☐									
8	☐									
9	☐									

Figure 7: *Diffuser* tab populated with example diffuser configuration.

5.2.3 Effluent characteristics

Effluent characteristics consisting of flow rate, temperature, and salinity play an important role in determining the behavior of the effluent plume and initial dilution at the culmination of nearfield mixing. The wastewater effluent flow rate may vary during the year based on water use whether it is industrial or municipal effluent. Similarly, effluent temperature may vary depending on the season, particularly for treatment plants with settling ponds that are exposed to varying air temperatures. Effluent salinity for municipal and industrial outfalls is typically zero. For existing outfalls, the effluent characteristics are typically set or selected based on analysis of available monitoring data. Higher flow rates cause stronger jet mixing but also deliver a large volume/mass and correspondingly have less dilution during subsequent phases. Conversely, lower flow rates provide lower jet mixing, but with a smaller volume/mass to mix, resulting in more dilution in turbulent mixing with ambient currents. In most situations, a combination of high effluent flow during low ambient currents results in the lowest dilutions. Regulatory guidance varies from state to state on how to select effluent characteristics. Most guidance documents suggest setting a combination of effluent flow rate, temperature, and salinity that would result in lowest dilutions, representative of critical conditions.

Click the *Effluent* Tab to enter input data related to effluent characteristics. The user also has an option to load previously saved effluent characteristics. Click the '*Load'* button to load the "Effluent_example.csv" file. Figure 8 shows loaded effluent characteristic values. Here the user also has the option to enter pollutant concentrations for two constituents of concern for mixing zone compliance evaluation. The example is a freshwater discharge at 8 million gallons per day (MGD) and has a temperature of 26.3°C. Only one pollutant is entered with a concentration of 100 mg/L. PLUMES2.0 will

simulate all pollutants as conservative pollutants, meaning the pollutant concentration is only altered upon discharge by dilution in the ambient receiving water, unless a decay rate is entered on the *Ambient* tab (described in the next Section).

Also shown under the *Effluent* Tab is a table to enter data related to Mixing Zone dimensions. Figure 8 also shows a schematic representation of acute and chronic mixing zone for a single port outfall. Mixing zone requirements vary by state and are established in state water quality standards regulations. For the example case in the PLUMES2.0 package, the selected mixing zones are chronic mixing zone = 102 m, and acute mixing zone = 10.2 m. Mixing zone dimensions may also be loaded from a prior saved file. Click the *Load* button to see to see the "Mixing_Zone_Example.csv" file.

Click the "case" buttons for the effluent characteristics and mixing zone characteristics to select the case of interest before moving to the *Ambient* tab.

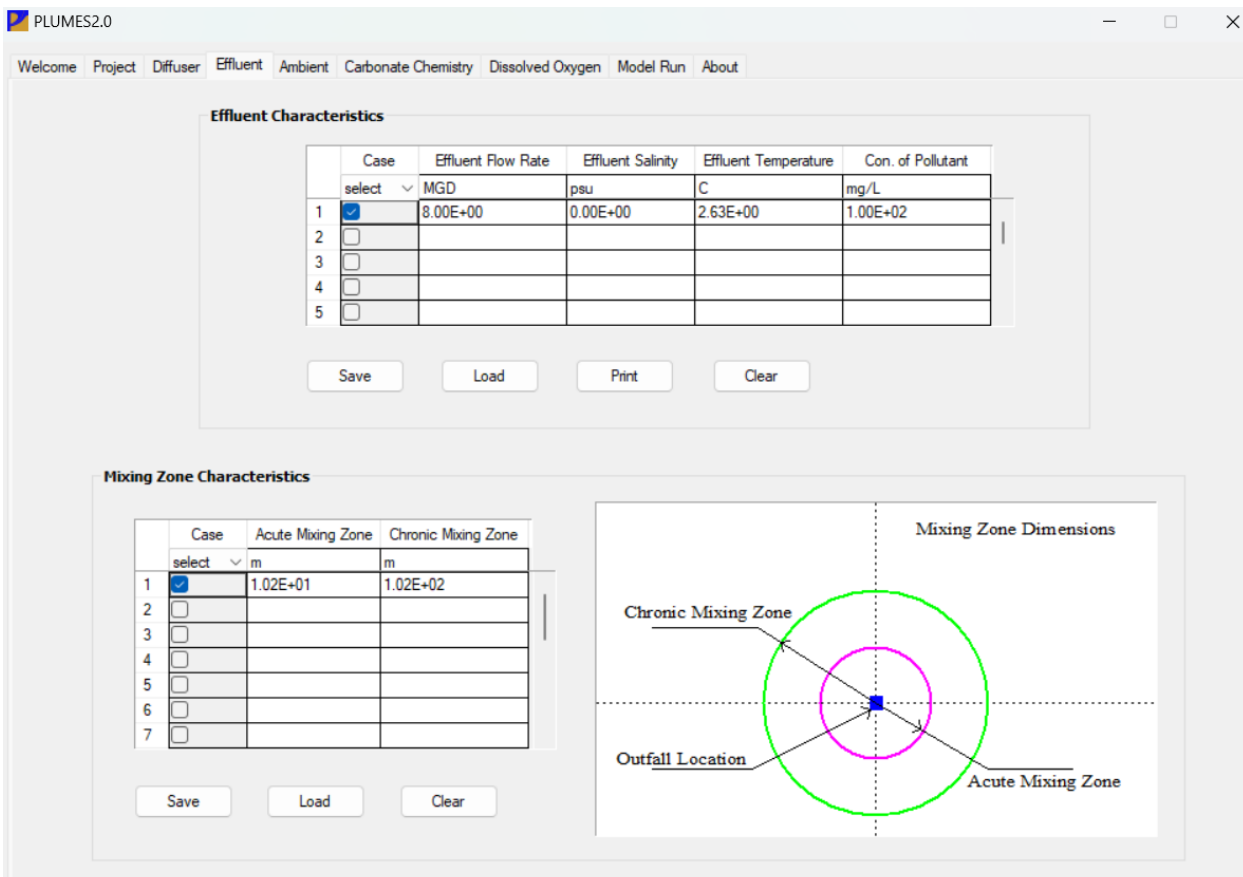


Figure 8: *Effluent* tab populated with example effluent characteristics.
The flow rate units may be million gallons per day (MGD), cubic meters per second (cms), or cubic feet per second (cfs). Temperature units may be °C or °F. Concentration of pollutants may be in units of mg/L or kg/kg of effluent.

5.2.4 Ambient characteristics

Ambient characteristics are the receiving water properties near the outfall discharge. Specifically, PLUMES2.0 requires entry of properties that affect the mixing and dilution of the effluent plume. They include ambient currents and stratification defined by temperature and salinity profiles. Strong ambient currents lead to faster dilution through entrainment mixing. However, in some situations, results may be counterintuitive. Stronger currents could also mean that the plume and the effluent are transported rapidly to the mixing zone boundary before the dilution process is completed, with lower initial dilution values (D) than expected. Similarly, strong stratification may result in trapping the plume lower in the water column, terminating the buoyancy-induced mixing. Lack of stratification may result in rapidly surfacing plume, in which case initial dilution may be limited by water depth. To account for such possibilities, regulatory agencies will run multiple scenarios under the range of expected ambient conditions to address the possibility that, for stratified waterbodies, the worst-case conditions could occur at either maximum or minimum stratification and during both low and high current speeds.

Figure 9 provides a schematic representation of a water column cross-section with salinity, temperature, and velocity-profiles near a submerged outfall defining the ambient input data needed for setting up a project run. The figure shows U (x-component of velocity), T (temperature, °C), and S (salinity) plotted as a function of depth (measured positive from the water surface).

The *Ambient* tab (see Figure 10) includes columns to enter velocity magnitude and direction, temperature, and salinity data as water column profiles. Note that nearfield velocity column represents velocity profile at the diffuser site. Farfield velocity profile represents currents to be used by the model for farfield transport and dilution calculations which may be different from currents at the diffuser location. Often nearfield and farfield current profile are the same, but it is not uncommon see applications where tidally averaged current velocities are entered for farfield transport when the calculations are to be conducted over large distances and over multiple tidal cycles. As explained in the introduction, the final concentration of the pollutant after dilution is affected by the background concentration of the pollutant. The background concentration may be a natural condition or impacted by pollution from upstream sources. These values may be entered under the *Backg.Con* column. If the pollutant is conservative then there is no decay, but if the pollutant concentrations diminish with time, then a decay rate may be entered in the column under *Pollu.Decay.* For example, if the pollutant is fecal bacteria, then a die-off rate of ≈ 1/day may be entered as a preliminary default value based on median value from several studies (US EPA, 1985).

The last three columns on this page are data needed for conducting farfield dilution calculations using the Brooks' method. They include the farfield velocity profiles – magnitude and direction (these may be the same as nearfield), and α (*alpha*) that is used to compute initial eddy diffusivity ϵ_o in the Brooks farfield transport and dilution equations. Initial diffusivity is a function of initial plume width w_o and is defined by the equation below.

$$\epsilon_0 = \propto \cdot (w_o)^{\frac{4}{3}} \tag{15}$$

where, $\propto$ may vary from 0.0001 $m^{2/3}s^{-1}$ to 0.0005 $m^{2/3}s^{-1}$. A standard value of $\propto$ =0.0003 $m^{2/3}s^{-1}$ is the recommended default, suitable for most cases (Brooks, 1960).

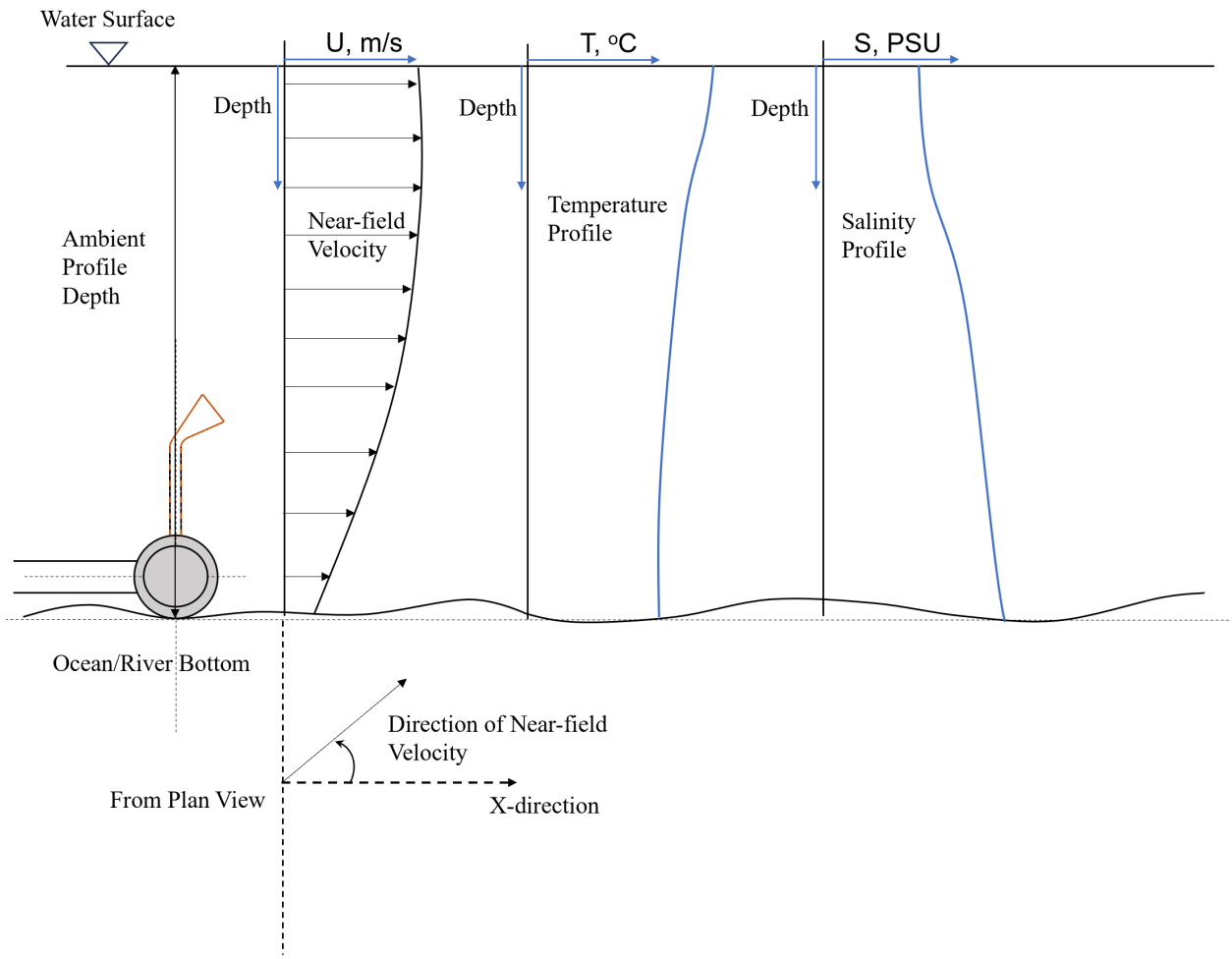


Figure 9: Schematic representation of ambient cross section near an outfall diffuser.

Click the *Ambient* Tab to enter input data related to ambient characteristics. The user also has an option to load a previously saved ambient characteristics. Click the *Load* button to see "Ambient_example.csv" file. Figure 10 shows loaded ambient characteristic values. In this example, the velocity profile shows currents varying in magnitude from 0.09 m/s at the surface to 0.05 m/s near the bottom. The current direction is 0°, so the current flows parallel to the shoreline (x-direction). The temperature profile shows warm temperatures of 14°C at the surface with a thermocline at 4 m depth, below which the temperatures are uniform at 8°C. Ambient salinity is 32 psu, uniformly distributed with depth. The farfield velocity field is populated with constant values of 0.05 m/s also flowing in the x-direction, the eddy diffusivity is set at the default α of 0.0003 $m^{2/3}$. Farfield calculations using Brooks' method assume constant ambient conditions, and the model determines those conditions based on the depth of the plume when the initial dilution ends (surface or plume trapping depth).

The user can visualize the *Ambient Profile* data by clicking the desired plot. Entered values may be saved as *.csv files for future use.

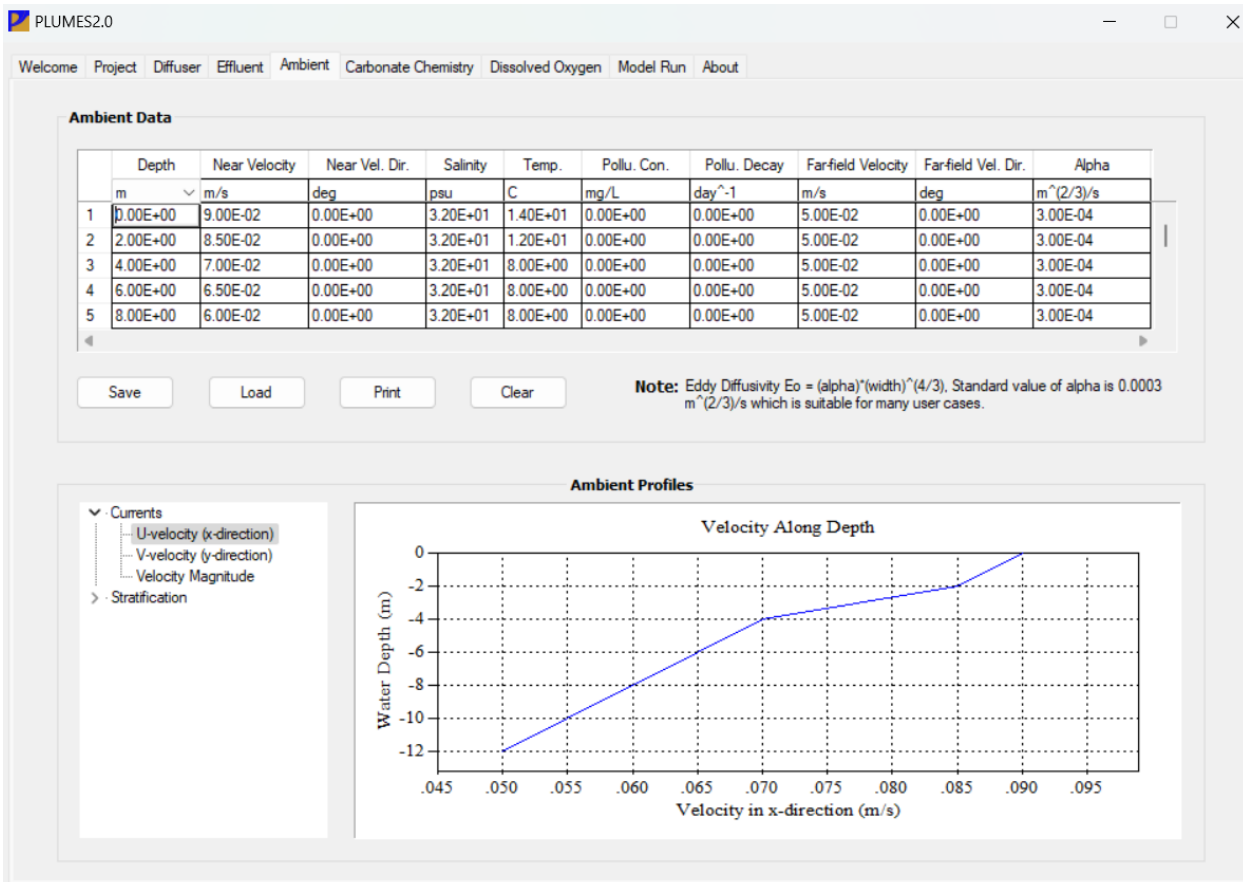


Figure 10: *Ambient* tab populated with example receiving water characteristics.

5.2.5 Carbonate chemistry – and pH calculation

Carbonate chemistry calculations are an added optional feature. Users may skip this tab and proceed directly to the *Model Run* tab (section 5.2.7) and initiate dilution simulations.

For computation of pH, TA, and DIC kinetics in the mixing zone, click the *Carbonate Chemistry* tab and check the box in the upper left corner titled "Calculate Carbonate Chemistry". This opens the dialogues which allow entry of effluent and ambient characteristics.

For carbonate chemistry calculations to proceed, only two of the three variables (pH, TA, and DIC) are needed. Typically, discharge monitoring reports or effluent characterization studies do not include DIC, but TA and pH are more readily available. Figure 11 shows an example of a high alkalinity effluent with a of pH = 8.9, TA of 2930 µmol/kg, and DIC of 2,500 µmol/kg. Users must update these to reflect their own effluent properties. Users must also provide ambient profiles of pH, TA, DIC and Ca^{2+}. The user also has an option to load a previously saved ambient characteristics. Click the *Load* button to select "AmbientChem_example.csv" to populate the ambient carbonate chemistry fields as shown in Figure 11.

The fields K1K2 and KSO4 representing dissociation constants for carbonic and sulfuric acid are also filled out with default selection of the temperature and salinity dependent relationships. The user has the choice to select from ten different options for K1K2 and four options for KSO4 for fine tuning the

model performance to best match site specific conditions. Similarly, dissociation constant(s) K for aragonite and calcite forms of calcium carbonate, and the reaction order for the purpose of computing saturation levels and precipitation rates are pre-filled out. As mentioned in Section 3.2, users may choose to change these parameters derived for site specific or updated experimental/laboratory data.

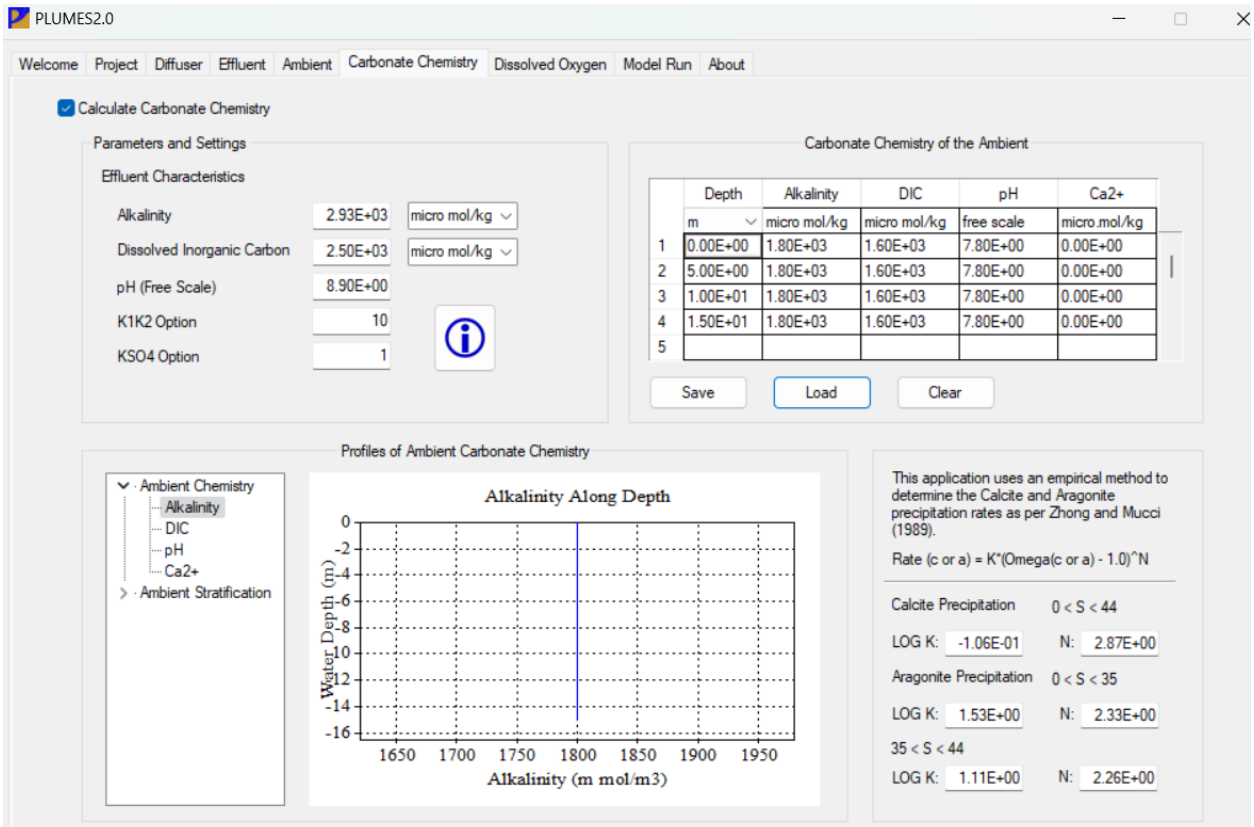


Figure 11: Carbonate Chemistry tab populated with example effluent and ambient water characteristics.

Use the *Model Run* tab to execute a run (section 5.2.7). When the model is run with carbonate chemistry calculations included, the text output automatically includes TA, DIC, pH, and aragonite and calcite saturation states - Ω_{arag}, Ω_{calc}. The output also includes precipitation rates for aragonite and calcite.

*<u>Note</u>: Unlike standard dilution model runs, the project file does not save carbonate chemistry information. However, the ambient carbonate chemistry values may be saved as *.csv files for future use.*

5.2.6 Dissolved Oxygen and Biochemical Oxygen Demand

The simulation of DO and BOD kinetics are also an added optional feature. Users may skip this tab and proceed directly to the Model Run tab and initiate dilution simulations.

Like the carbonate chemistry calculations, DO and BOD concentrations in effluent as well as the ambient waters must be determined by the user based on available data as part of effluent and receiving water characterization and provided as input. Click the *Dissolved Oxygen* tab and check the box in the upper left corner titled "Dissolved Oxygen Calculations". This opens the dialogues which allow entry of

effluent and ambient characteristics. The effluent characteristics field have been populated with an effluent with low DO of 2.0 mg/L, IDOD of 0.0 mg/L and $cBOD_5$ and $nBOD_5$ levels of 30 mg/L and 20 mg/L. These values must be replaced by the effluent characteristics determined by the user. The $cBOD_5$ and $nBOD_5$ decay rates based on US EPA (1994) may be treated as default values but could be updated with site/effluent specific information.

Users must also provide ambient profiles of DO, $cBOD_5$, and nBOD5. The user also has an option to load previously saved ambient DO-BOD characteristics. Click the *Load* button to select "AmbientDO_example.csv" to populate the ambient DO-BOD fields as shown in Figure 12 below.

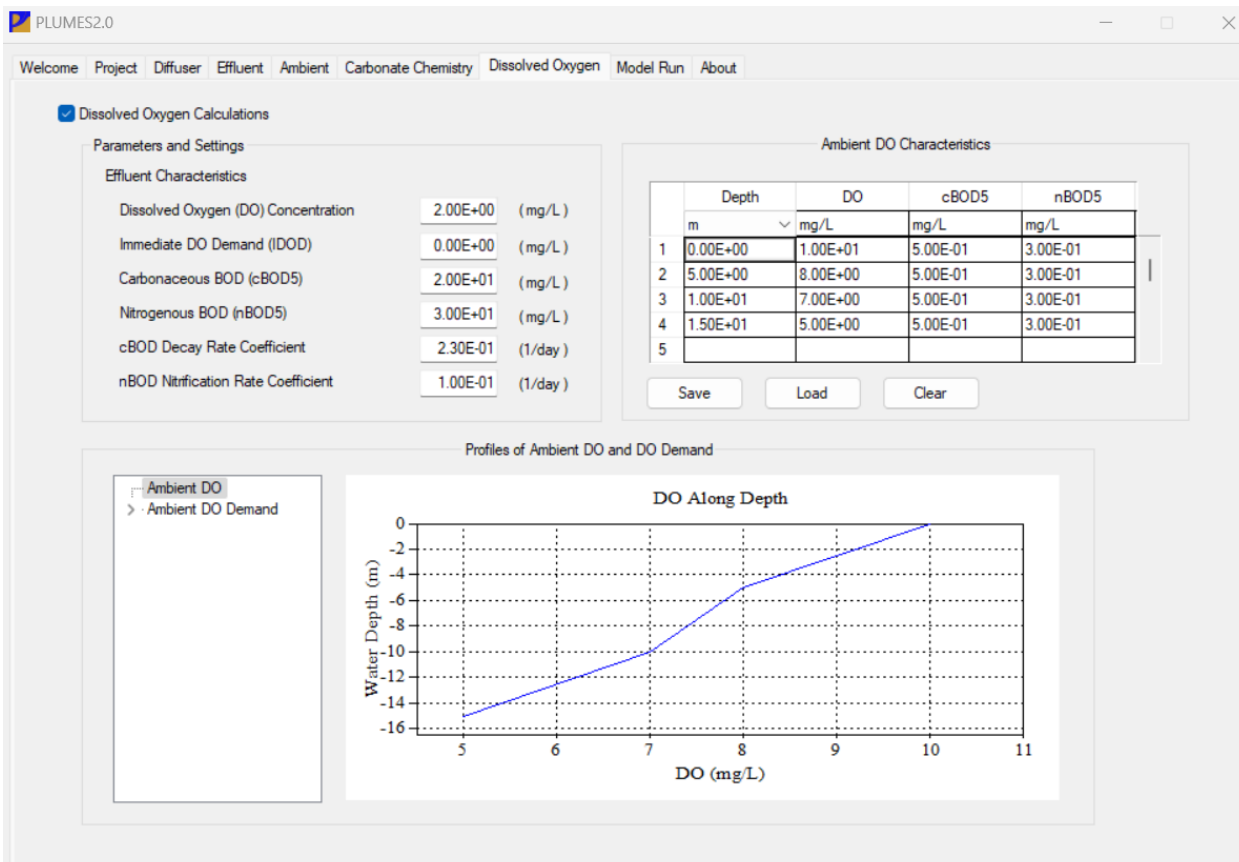


Figure 12: Dissolved Oxygen tab populated with example effluent and ambient water characteristics.

Use the Model Run tab to execute a run (section 5.2.7). When the model is run with DO calculations included, the text output automatically includes DO concentrations in the text output.

*<u>Note</u>: Unlike standard dilution model runs, the project file does not save DO-BOD information. However, the ambient DO-BOD values may be saved as *.csv files for future use.*

DO and pH calculations cannot be conducted simultaneously and must be done as independent runs. In other words, "Dissolved Oxygen Calculations" and "Calculate Carbonate Chemistry" boxes cannot be checked/selected for the same model run.

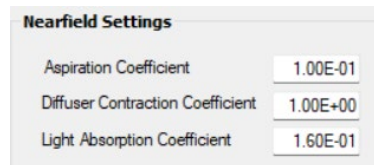
5.2.7 Model Run

Once the diffuser, effluent, and ambient data entry are completed, the final model run settings may be selected and a dilution run initiated. Click the *Model Run* tab to enter the nearfield and farfield settings. For convenience, many of the menu items are pre-selected or pre-filled with default values.

Under the Nearfield Setting tab, the following three entries are pre-filled with default values (same values as Visual Plumes defaults for UM3; see insert below or Figure 13).

- Aspiration coefficient: The aspiration coefficient specifies the rate at which ambient fluid is entrained into the plume. The default value of 0.1 is an average value that has been commonly used. A different value causes increases or decreases in plume spreading and affects other characteristics, like plume rise.

- Diffuser contraction coefficient: Users may specify a contraction coefficient (reduction in area of the jet relative to the port area) based on the type of discharge ports on the diffuser. The discharge coefficient of sharp-edged ports (cylindrical hole in the diffuser pipe wall) is about 0.61. For bell-shaped ports (flaring inward into the direction of flow), a value of 1.0 is usually used. The default value is 1.0.



- Light absorption coefficient (not used in current version of PLUMES2.0): This coefficient is provided as an option for future development. It is for specifying the light absorption coefficient for the Mancini bacteria model. This is the coefficient *ke* found in Mancini, 1978, that describes water clarity. The default value is 0.16.

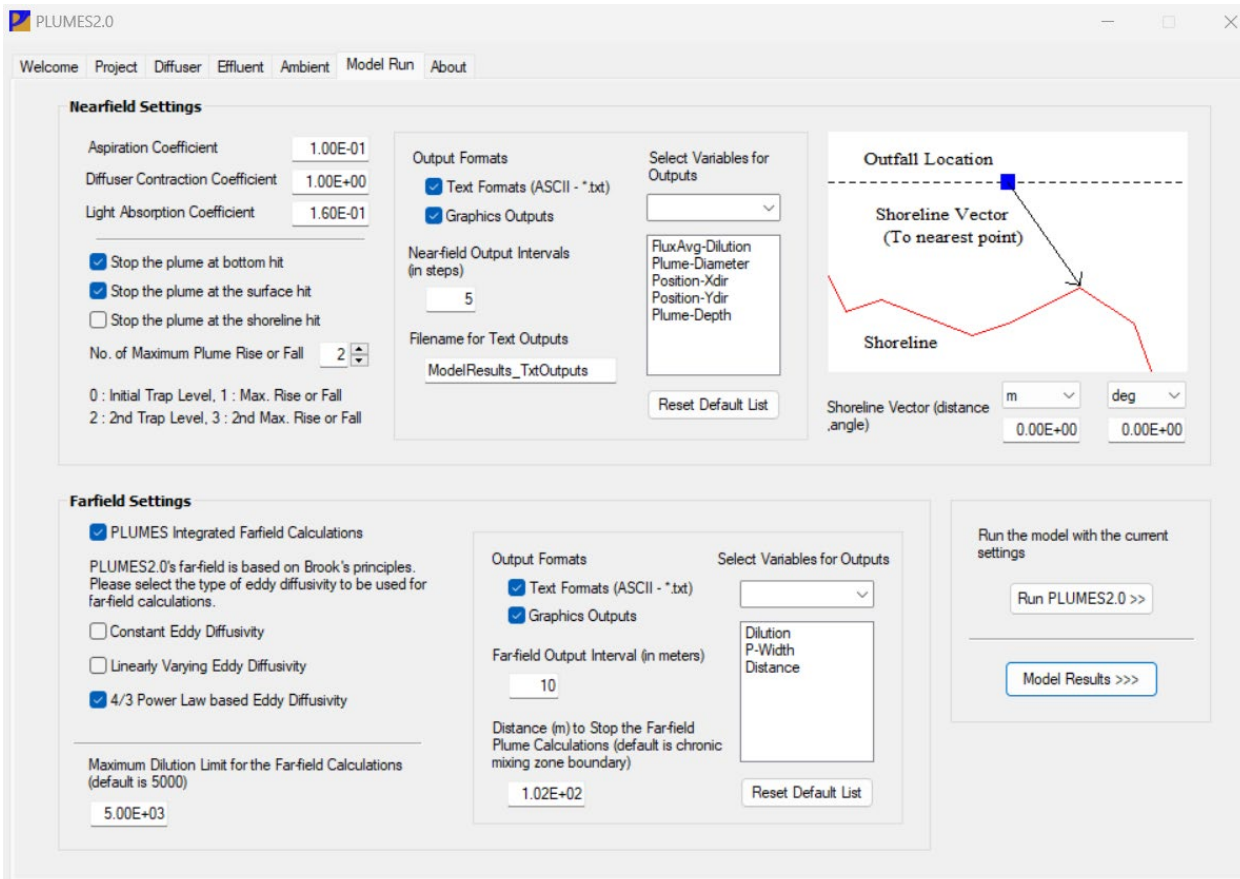


Figure 13: Model Run tab populated with example/default settings.

Here the user should also select the options that define termination of the initial dilution stage of calculations, based on impingement with boundaries including the bottom, free surface, shoreline, and/or trapping depth, by checking the suitable box(es). As shown in Figure 13, the boxes "Stop the plume at bottom hit" and the "Stop the plume at the surface hit" are checked as default. If these values are used, the initial dilution calculations will be terminated automatically if the plume surfaces or encounters the bottom. If the shoreline hit box is selected, then the model asks for the vector corresponding to the shortest distance to the shoreline from the diffuser. For atypical settings such as diffusers on a slope with downward facing ports, bottom impingement can occur immediately. The user must ensure that ambient water depth in such settings is significantly greater than the port depth.

Selection of "No of Maximum Plume Rise or Fall" (0, 1, 2, or 3) provides additional options to instruct the program when to terminate initial dilution and begin far-field calculations. In some situations, the plume may stabilize in the middle of the water column, or the user may wish to allow the calculations to continue beyond surface interaction (boil). When "0" is selected, initial dilution is terminated during the initial plume rise when the neutral buoyancy depth (initial trapping depth) is reached. When "1" is selected, the plume momentum is allowed to carry it beyond the initial trapping depth to its maximum rise in the water column. When the default value of "2" is selected, gravity allows the plume to settle back to a new neutral buoyancy depth (2nd trapping depth). When "3" is selected, the downward momentum allows the plume to sink deeper beyond the 2nd trapping depth to its maximum fall. For discharges with negative vertical angle of the discharge, the rise and fall sequence is reversed. As described in in Frick et al. (2003), under ideal conditions a plume will oscillate about a varying trapping level at the so-called Brunt-Väisala frequency as a wave form.

A schematic is shown on the top right panel of the tab with cells for entering distance and direction to the shoreline. The convention for the angle is +tive counter-clockwise from the x-axis. Under "Output Formats", the user may enter the selections for type of model output (ascii text or graphical). The "Select Variables for Outputs", with a dropdown menu, allows the user to add more variables to be included in addition those indicated in the default list. Model results are written to output files at a user-defined number of intervals (steps). This allows the user to add or reduce the output resolution. For the nearfield, the setting is based on internal model steps, and the highest resolution is setting the interval = 1 (model step). The default value in the model is set at 5.

Under the farfield settings section, the user may select linked computation of nearfield and farfield dilution by checking the box next to PLUMES Integrated farfield calculations (already checked as default). By doing so, the model transitions automatically from the nearfield phase to the farfield phase, using the projected area calculations to determine the initial wastefield width, and initiates the Brooks method for farfield dilution calculations. Depending on the nature of the ambient waterbody, the user may select (a) Constant Eddy Diffusivity (for rivers and narrow channels), (b) Linearly Varying Eddy Diffusivity (for estuarine condition), or (c) Eddy Diffusivity Variation based on Brooks 4/3rd law (for open ocean conditions, checked as default) (Table 2).

This tab also provides an option to limit Maximum Dilution (a high value such as 5000:1, default) or distance values (such as chronic mixing zone length or user-defined distance beyond the study area of interest) to terminate the farfield calculations. As in the nearfield menu, the user may select variables to be printed in addition to those listed as default and select text or graphical output formats (or both).

For the farfield model, the output interval is in meter units, and the default is set at 10 m. A larger number for the interval (steps for the nearfield and meters for farfield) results in lower spatial resolution but a shorter printout. The user may also enter the file name for the model results output file to be saved in the project directory.

Once the model inputs are completed, click the *Model Run* button to initiate the model run. If the inputs are complete and the model runs without errors, a message "Model run was completed successfully!" is displayed.

5.2.8 Model Results

The results are saved in the filename provided in the box under "Filename for Text Outputs" on the *Model Run* page. In this example the filename provided was "ModelResults_TxtOutputs". After the model runs, click OK to close the dialogue box indicating message "Model run was completed successfully!". At the lower right corner of the *Model Run* tab, a new *Model Results* tab becomes available following the completion of model run. Click the *Model Results* to see Graphic Outputs. Slide the Graphic Outputs window and move it to a side to see the Text Output window hidden behind.

The text output organization was deliberately designed to be identical to the output file that users are familiar with from the Visual Plumes interface (see Figure 14). The Ambient Table and Diffuser Table summarize user-provided inputs for the scenario. Simulation Results are provided immediately below. The results are written in rows at the indicated model steps. The default output columns include (1) Flux-averaged Dilution, (2) Plume Diameter, (3) and (4) x- and y- coordinates of the plume centerline, (5) Plume depth relative to water surface. Optional user-specified output parameters included in the example in Figure 12 were (6) Plume salinity, and (7) Pollutant concentration. Note that the results are only presented in metric system of units.

In this example, the buoyant plume rises in the water column and is also carried away in the x-direction by the ambient currents. The plume dilution increases with each step as the plume rises all the way to the water surface. In this example, the upward momentum of the plume carries it past the trapping depth to the surface, and the calculations are terminated when the plume outer boundary touches the water surface [see Figure 15(a)]. As shown in the text output in 14, this occurs when the plume upward momentum has carried it beyond the initial trapping depth of 3.0 m to a (plume centerline) depth of 2.5 m below the surface when the outer boundary of the plume touches the water surface. The volumetric dilution of the plume at this stage is 169.8:1.

If the user had unchecked the "Stop the plume at the surface hit", the upward momentum would have carried the plume to the boil-over stage to a maximum centerline elevation, a depth of 1.9 m. This distance is less than the plume diameter (≈7.8 m in this case) indicating the formation of a plume boil, and with a higher initial dilution of 185:1. With the "No. of Maximum Plume Rise of Fall" switch set at the default value of 2, the plume calculations continue. The plume reverses direction and falls back to the second trapping depth of 3.4 m. The plume at this stage is further away from the diffuser and at a higher initial dilution of 217:1. Note that caution is advised when using the model beyond the boundary interaction point (surface hit), because the model over-simplifies the complex mixing in a plume boil.

Back to the Figure 13 example, having checked PLUMES Integrated Farfield Calculations and Brooks 4/3rd Power Law for Eddy Diffusivity, the computations transition automatically to the farfield phase. The farfield calculations begin with two key, internally calculated wastefield characteristics: (1) starting dilution of the wastefield after initial dilution, 169:8, and (2) the width of the wastefield in the direction of the current (note that this will represent the width of merged plumes from a multiport diffuser). This internally computed value is based on final multiple merged plumes at the termination of initial dilution dimensions, affected by current direction and diffuser configuration (109 m in this example).

Results shown in Figure 14 indicate that, at 100 m, just before the specified 102 m mixing zone, flux averaged dilution of the plume is 179.5:1 and the wastefield is 129.5 m wide. To see the result at the exact 102 m distance, the user must set the farfield output interval to 1 m instead of the 5 m interval used in the example. Using 1 m interval, at the 102 m mixing zone, the flux averaged dilution of the plume is 180.1:1 and the wastefield width is 130.3 m wide

In the Graphic Outputs window (see insert), the user can choose to explore numerous visualization options that are available. Two examples are provided below.

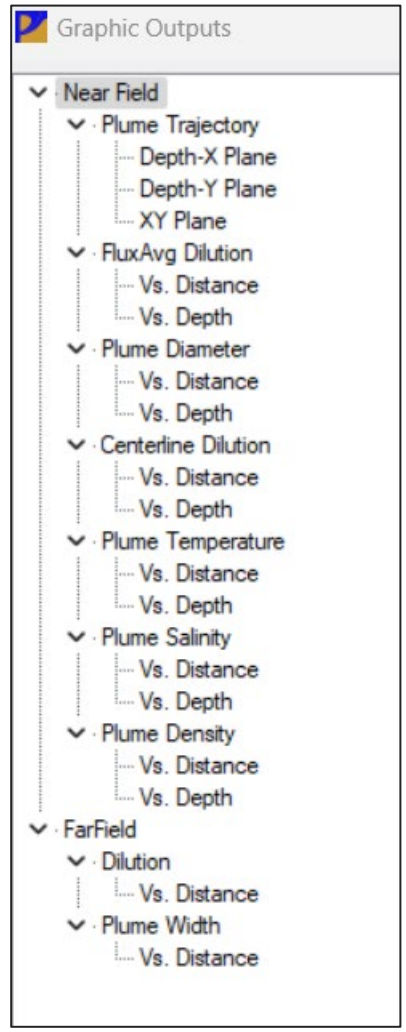
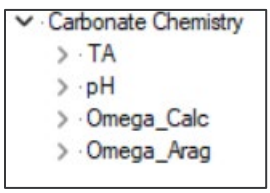
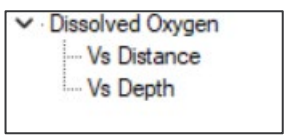


Figure 15 shows plots of the plume trajectory in x-y or Depth-X plane. Figure 15 (a) corresponds to the case when plume calculations were allowed to go past the surface impact and shows the plume boiling over. Figure 15 (b) corresponds to the case when the plume calculations were terminated at surface impact (consistent with the example project).

As shown in the insert to the right or in Figure 13, there are many plotting options available to the user for examining various plume properties such as Plume (flux averaged) Dilution, Plume Diameter, Plume (centerline dilution), Temperature, Salinity, and Density.

Options for visualizing plots of carbonate chemistry variables pH, TA, and Ω_{arag} and DO become available if the model is run with carbonate chemistry or dissolved oxygen calculations switched on.





Example plots for carbonate chemistry variables and DO concentrations as a function of distance from the outfall are shown in Figure 16 (a) and (b) respectively.

```
*****************************************************************************************
-----------------------------------------------------------------------------------------
Ambient Table:
     Depth   Amb-cur   Amb-dir   Amb-sal   Amb-tem   Amb-pol     Decay   Far-spd   Far-dir   Disprsn
       (m)     (m/s)     (deg)     (psu)       (C)    (mg/L)   (1/day)     (m/s)     (deg)(m0.67/s2)
     0.000     0.090     0.000    32.000    14.000     0.000     0.000     0.050     0.000   0.00030
     2.000     0.085     0.000    32.000    12.000     0.000     0.000     0.050     0.000   0.00030
     4.000     0.070     0.000    32.000     8.000     0.000     0.000     0.050     0.000   0.00030
     6.000     0.065     0.000    32.000     8.000     0.000     0.000     0.050     0.000   0.00030
     8.000     0.060     0.000    32.000     8.000     0.000     0.000     0.050     0.000   0.00030
    10.000     0.055     0.000    32.000     8.000     0.000     0.000     0.050     0.000   0.00030
    12.000     0.050     0.000    32.000     8.000     0.000     0.000     0.050     0.000   0.00030
-----------------------------------------------------------------------------------------
Diffuser Table:
     P-dia    P-elev   V-angle   H-angle     Ports   Spacing   AcuteMZ   ChrncMZ   P-depth   Ttl-flo
       (m)       (m)     (deg)     (deg)       ( )       (m)       (m)       (m)       (m)     (MGD)
      0.08      0.31     45.00     30.00     18.00      6.10     10.20    102.00     11.00      8.00
-----------------------------------------------------------------------------------------
Simulation Results:
            Dilutn     P-dia    x-posn    y-posn     Depth        DO
      Step (FluxAvg)     (m)       (m)       (m)       (m)    (mg/L)
        10     1.213    0.091     0.024     0.014   -10.972     2.719
        20     1.474    0.111     0.054     0.031   -10.938     3.419
        30     1.791    0.135     0.089     0.051   -10.898     3.996
        40     2.178    0.164     0.133     0.076   -10.848     4.472
        50     2.650    0.199     0.185     0.105   -10.789     4.867
        60     3.225    0.242     0.249     0.141   -10.717     5.195
        70     3.926    0.293     0.326     0.183   -10.631     5.470
        80     4.780    0.355     0.419     0.233   -10.528     5.702
        90     5.822    0.430     0.530     0.292   -10.405     5.901
       100     7.092    0.518     0.663     0.360   -10.259     6.073
       110     8.640    0.624     0.820     0.440   -10.085     6.225
       120    10.527    0.747     1.007     0.531    -9.879     6.363
       130    12.827    0.892     1.225     0.633    -9.636     6.485
       140    15.631    1.059     1.476     0.747    -9.351     6.594
       150    19.049    1.250     1.758     0.867    -9.024     6.694
       160    23.215    1.467     2.069     0.992    -8.654     6.789
       170    28.294    1.713     2.407     1.118    -8.241     6.881
       180    34.485    1.988     2.771     1.244    -7.782     6.971
       190    42.032    2.298     3.162     1.367    -7.278     7.063
       200    51.232    2.644     3.583     1.486    -6.726     7.156
       210    62.446    3.031     4.035     1.600    -6.126     7.254
       220    76.117    3.463     4.525     1.708    -5.475     7.356
       230    92.781    3.947     5.057     1.811    -4.775     7.464
       240   113.094    4.486     5.639     1.907    -4.024     7.596
       250   137.648    5.144     6.256     1.994    -3.263     7.758
-------------------------- Plume traps --------------------------
------------------------- merging happened --------------------------
       260   155.017    5.722     6.621     2.038    -2.869     7.869
       270   165.961    6.243     6.894     2.069    -2.614     7.936
-------------------------- Plume surfaces -----------------------
       275   169.754    6.481     7.017     2.082    -2.512
------------------- Starting Farfield Calculations -------------------
Farfield dispersion based on wastefield width of :      96.29 (m)
4/3 Power Law based Eddy Diffusivity is used:
  Dilution      Width  Distance      Time        DO
       ()        (m)       (m)    (hrs.)     (mg/L)
   169.754    98.151    10.000     0.031      7.939
   169.754   101.535    20.000     0.088      7.899
   169.765   104.925    30.000     0.143      7.880
   169.888   108.344    40.000     0.199      7.842
   170.321   111.796    50.000     0.255      7.807
   171.211   115.278    60.000     0.310      7.792
   172.605   118.791    70.000     0.365      7.766
   174.483   122.335    80.000     0.421      7.756
   176.793   125.910    90.000     0.476      7.738
   179.479   129.517   100.000     0.531      7.724
............................ Reached Chronic Mixing Zone .............
   180.792   131.144   104.484     0.556      7.724
```

or using 1 m Far-field Interval

```
   179.491   129.532   100.000     0.532      7.724
   179.779   129.894   101.000     0.537      7.724
............................ Reached Chronic Mixing Zone .............
   180.070   130.258   102.000     0.543      7.724
   180.364   130.621   103.000     0.548      7.724
   180.661   130.985   104.000     0.554      7.724
   180.792   131.144   104.438     0.556      7.724
```

Figure 14: Example of ascii text format output from PLUMES2.0.

Initial dilution was terminated when the plume boundary encountered the water surface, when the plume centerline was at a depth of 2.4 m below the water surface at an initial dilution of 169:1. The far-field calculations began at this point with a merged wastefield width of 109 m. The far-field calculations were terminated at the Chronic Mixing Zone boundary (102 m). The dilution of the plume at this distance was 176:8.

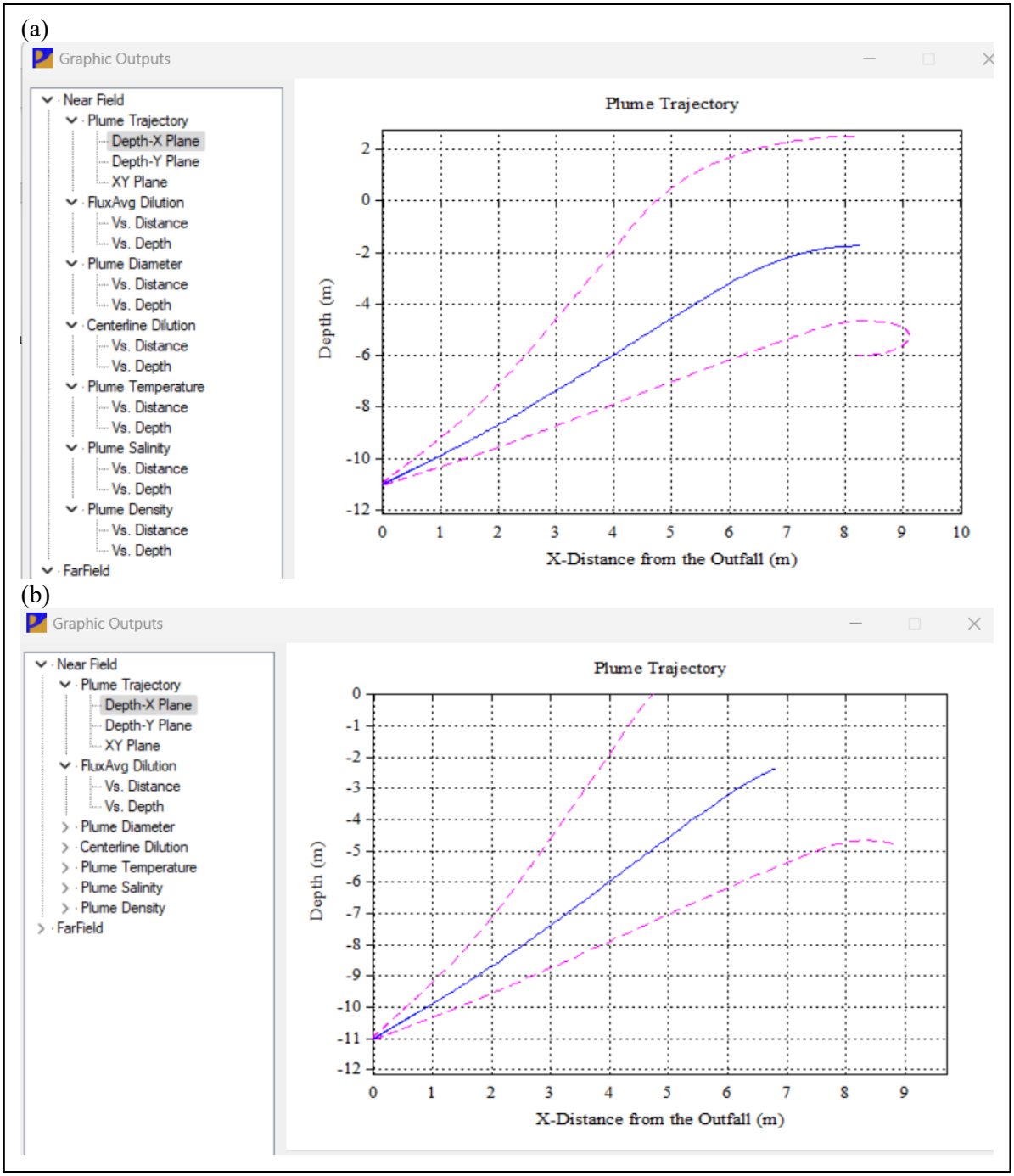


Figure 15: Example of plume trajectory in Depth-x plane until the termination of initial dilution phase.
(a) Initial dilution is allowed to continue past surface hit to completion of the boil;
(b) initial dilution is terminated at surface hit.

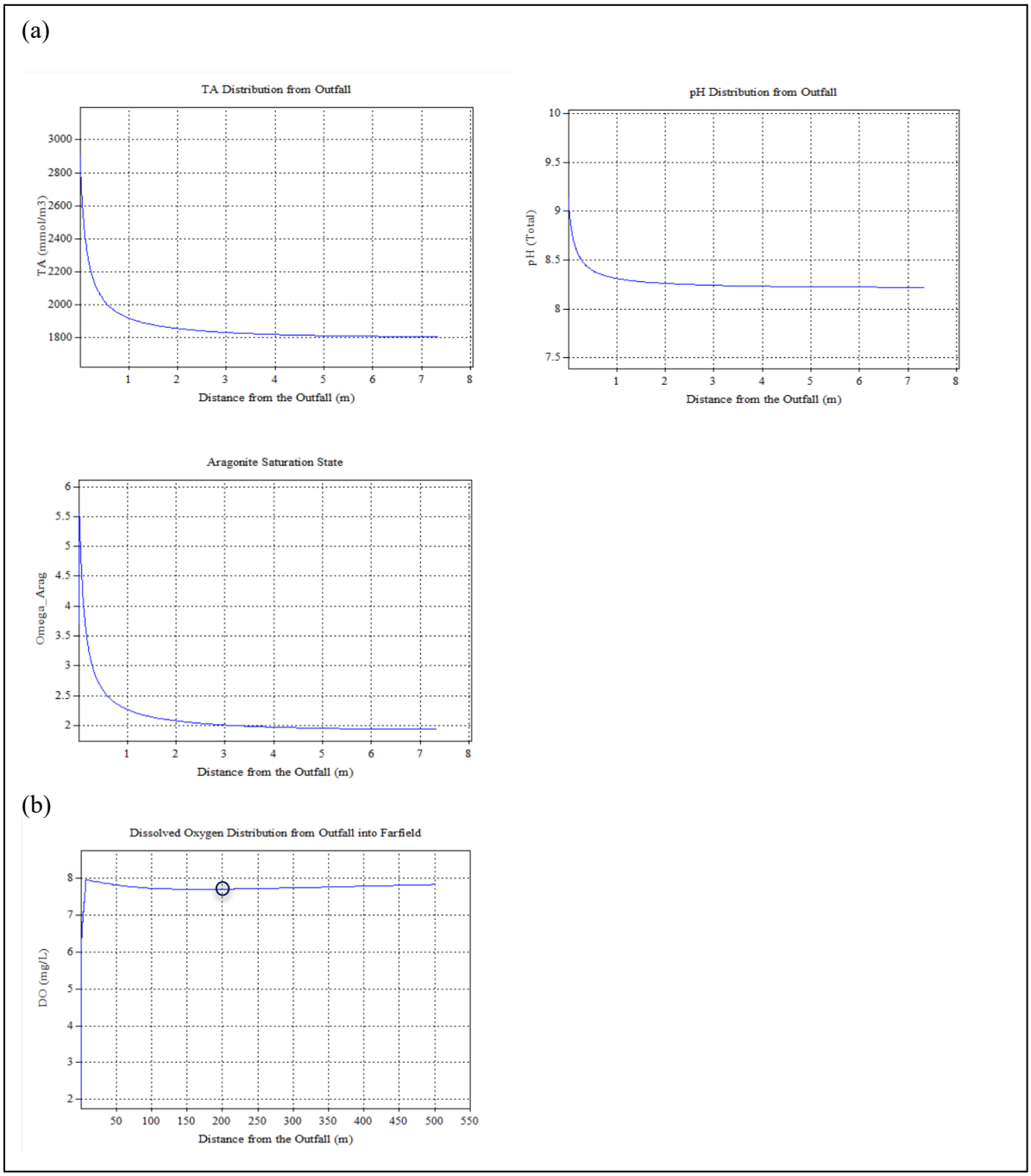
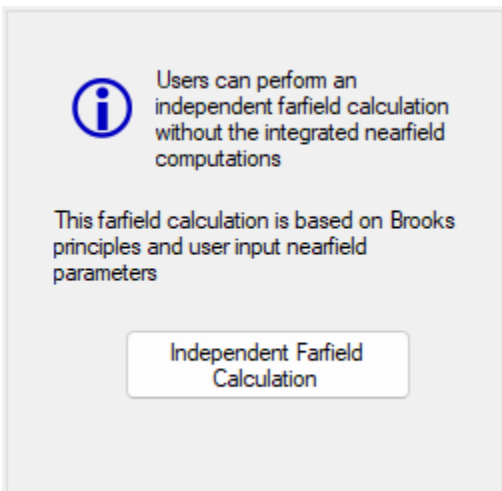


Figure 16: (a) Example plots of TA, pH, and Ω_arag within the nearfield zone of initial dilution zone.
The concentrations drop rapidly due to the initial dilution process.
(b) DO levels after initial dilution and subsequent sag (minima) in the far-field approximately 200 m away from the outfall.

5.2.9 Independent Far-field Calculation

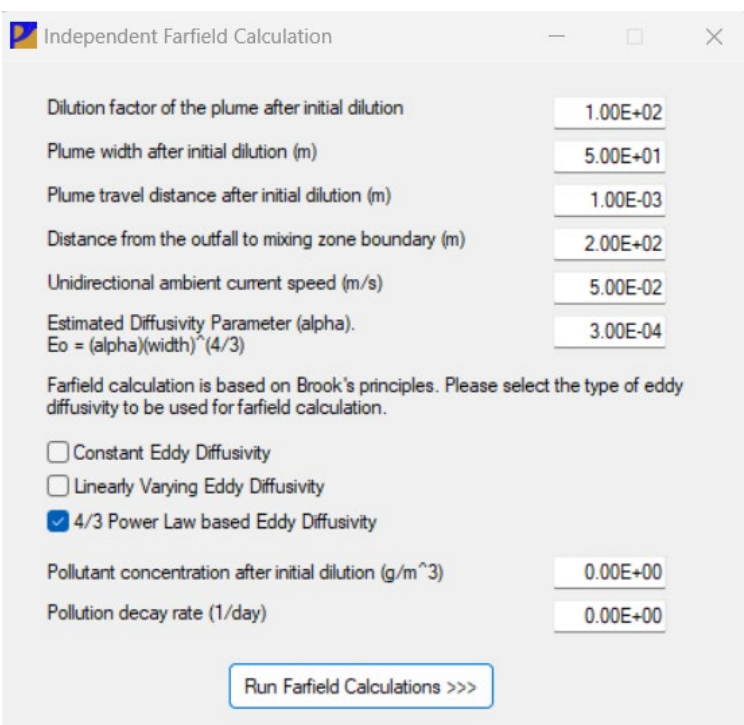
There are many instances where effluent transport and mixing in the surface waters occurs without the benefit of nearfield mixing provided by an outfall diffuser. A wastefield may form because of discharges from multiple sources, irregularly distributed in a localized area. The wastefield may then be carried away by ambient currents being diluted by farfield mixing processes. Conventional use of a dilution model such as PLUMES2.0 is not feasible in such instances. However, transport and dilution of the wastefield may be estimated through independent application of Brooks' laws.



To facilitate use of the model for such situations, we have included the Independent Farfield Calculation option. This can be accessed from the *Project* page. The only inputs required are (a) *Initial wastefield dilution* (existing dilution ratio at the start of farfield transport), (b) *Initial wastefield width*, (c) *Initial wastefield location* (distance from the outfall), (d) *Mixing zone location* (distance from the outfall), and (e) *Ambient current velocity*.

If Initial wastefield dilution is known, then the Brooks' calculations provide the combined Farfield dilution as a function of distance travelled. If the initial dilution is unknown, the users may enter 1 (a conservative approach assuming no dilution of the effluent in the wastefield at the start of farfield calculations). The Brooks' calculations then provide a relative farfield dilution factor.

Click the Independent Far-field Calculation button. This opens a new dialogue box. It is not possible to save the settings of the Independent far-field calculations, so the user must input values each time.



In this example, *Initial wastefield dilution* was set at 100:1. *Initial wastefield width* was set at 50 m. The *Initial wastefield location* was set to 0.001 m. (note this value can be as small as 0.001m but not zero). The mixing zone boundary was set at 200 m from the outfall. The unidirectional ambient current speed (same as Farfield velocity) was set at 0.05 m/s. The value of α that is used to estimate initial Eddy Diffusivity of the wastefield is set at 0.0003 as a default. Results for this example are shown in Figure 14 below.

The user has the option to select the variation of Eddy Diffusivity based on the environment. Typically, Constant Eddy diffusivity is selected for rivers and bounded channels, Linearly Varying Eddy diffusivity is recommended for estuarine settings, and Brooks' 4/3rd

power law variation is recommended for open ocean conditions. The user has the option to specify the Initial Concentration of the Pollutant in the wastefield, and a decay rate if applicable. Click the Run Farfield Calculations button to initiate the Independent Farfield Simulation. The text output results open in a new window and must be saved by clicking the File and Save as options.

In its present state of development, the user does not have control over the output interval in the independent farfield calculator. The calculator divides the user-defined distance to the mixing zone boundary into 25 steps, and 3 additional steps beyond the mixing zone boundary are included in the output. In the example above, the distance to the mixing zone boundary (200 m) is divided by the fixed number of output steps (25) and the model outputs the dilution in 8 m intervals. Three additional steps past the mixing zone boundary result in the final model output at 224 m.

Results for this example are shown in Figure 17 below.

Text Outputs for Independent Farfield Calculation

File Edit Search

```
Farfield dispersion based on wastefield width of :      50.00 (m)
4/3 Power Law based Eddy Diffusivity is used:
-----------------------------------------------------------------
The alpha value used for dispersion calculation:     0.0003
The ambient current in the farfield (m/s):     0.0500
*****************************************************************
Simulation Results:
-----------------------------------------------------------------
```

Conc (kg/m^3)	Dilution ()	Width (m)	Distance (m)	Time (hrs.)
0.000	100.000	52.137	8.001	0.044
0.000	100.004	54.303	16.001	0.089
0.000	100.100	56.499	24.001	0.133
0.000	100.495	58.724	32.001	0.178
0.000	101.326	60.977	40.001	0.222
0.000	102.609	63.258	48.001	0.267
0.000	104.294	65.567	56.001	0.311
0.000	106.319	67.903	64.001	0.356
0.000	108.625	70.266	72.001	0.400
0.000	111.163	72.657	80.001	0.444
0.000	113.894	75.073	88.001	0.489
0.000	116.786	77.516	96.001	0.533
0.000	119.816	79.985	104.000	0.578
0.000	122.965	82.480	112.000	0.622
0.000	126.216	85.000	120.000	0.667
0.000	129.559	87.545	128.000	0.711
0.000	132.984	90.115	136.000	0.756
0.000	136.483	92.709	144.000	0.800
0.000	140.049	95.329	152.000	0.844
0.000	143.678	97.972	160.000	0.889
0.000	147.365	100.639	168.000	0.933
0.000	151.106	103.330	176.000	0.978
0.000	154.899	106.045	184.000	1.022
0.000	158.740	108.783	192.000	1.067
0.000	162.627	111.544	200.000	1.111
0.000	166.559	114.328	208.000	1.156
0.000	170.534	117.135	216.000	1.200
0.000	174.550	119.965	224.000	1.244

Figure 17: Example of Far-field plume trajectory in -x direction.
Initial wastefield width was set to 109 m and ambient current carrying the wastefield or plume away from the source was 0.05 m/s.

6.0 Summary and Discussion

The Visual Plumes (UM3) model has been a workhorse for public domain mixing zone modeling for many years. The original Visual Plumes was a Windows-based computer application that superseded the DOS based PLUMES mixing zone modeling system. However, its availability and usability have waned in recent years due to compatibility issues with the latest versions of mandatory Windows upgrades. As a result, many users have been inconvenienced. SSMC scientists had developed a Fortran version of UM3 as part of the Salish Sea Model. The objective of this work was to take advantage of the preliminary development efforts by the SSMC scientists and develop, test, and release a new version of PLUMES (PLUMES2.0) along with a User's Manual. This goal has been accomplished with potential for future improvements such as addition of carbonate chemistry modules for pH and total alkalinity (TA) and simplified dissolved oxygen kinetics. Since then, the model development team has become aware of another (web based) public domain version of Visual Plumes UM3 offered by the San Francisco Estuary Institute and the Aquatic Science Center (SFEI 2024). The user community is therefore now well supported by two independent sources of public domain software based on the Visual Plumes suite of tools.

Simplicity and ease of use allow PLUMES2.0 model application to many complex problems. For example, simulation of dissolved oxygen (DO) or pH can be supported by PLUMES2.0 estimates of nearfield dilution to estimate concentrations prior to further biogeochemical or carbonate chemistry analyses. However, caution must be exercised as many settings will likely fall outside of the ideal combinations of diffuser geometries and receiving water conditions that were assumed in the development of the model formulations and numerical solutions. For example, the model assumes steady state and laterally uniform receiving water conditions with a cross flow. In stagnant environments or in tidally reversing currents, re-entrainment can occur. The actual dilutions of the effluent may be different from those provided by the model due to unsteady conditions and cumulative effects on ambient concentrations. Limitations of the model relating to boundary interaction were discussed previously. While the model provides options for the plume calculations to be terminated upon boundary impingement, experienced users may use the model beyond this limit with proper selections of eddy diffusivity and other parameters. Validation of model predictions using dye-dilution field studies is recommended while using PLUMES2.0 in complex and non-ideal settings. Similarly, although the model is designed to accommodate only regular geometry (e.g., linear diffuser with all ports in the same direction), experienced users can simulate irregular settings by breaking up the complex discharges into simpler geometries and using the principle of superposition. It is also important to note that the model was designed for simulating buoyant discharges. Discharge of brine or sediment loaded fluids heavier than ambient through PLUMES2.0 is possible by adjusting the density through T and S, but the model will terminate soon after the initial jet phase as the plume with water heavier than ambient begins to reverse before the initial dilution process is completed. Also, as discussed in Section 2.3.1, the model provides an estimate of centerline dilution, which is the minimum dilution for circular plumes with the understanding that dilution can vary significantly from near the port to the termination of initial dilution.

The addition of carbonate chemistry (TA, DIC, pH, and Ω_{arag}) into PLUMES2.0 was done at the request of user community engaged in alkalinity enhancement efforts to enhance marine CO_2 removal and mitigate ocean acidification. They may be used to design outfall and discharge strategies and to facilitate pH compliance assessments. The simplified DO calculations were added by the developers as they could be incorporated in a relatively straightforward manner for use by the community to conduct screening level DO impact assessments.

7.0 References

Abraham, G. 1963. Jet Diffusion in Stagnant Ambient Fluid. Publ. No. 23 Delft Hydraulics Laboratory July 1963.

Akar, P.J., Jirka, G.H., 1991. CORMIX2: An Expert System for Hydrodynamic Mixing Zone Analysis of Coventional and Toxic Multiport Diffuser Discharges. DeFrees Hydraulic Laboratory, School of Civil and Environmental Engineering, Cornell University, New York. EPA/600/3-91/073.

Baumgartner, D.J., Frick, W.E., Roberts, P.J.W., 1994. Dilution Models for Effluent Discharges. Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C.

Brooks, N.H., 1960. Diffusion of sewage effluentin an ocean current, in: Pearson (Ed.), Proceedings of the First Conference on Waste Disposal in the Marine Environment. Pergamon Press, New York, USA, pp. 246–267.

Cederwall, K. 1971. Buoyant slot jets into stagnant or flowing envirorment. Rep. No. KH-R-25. W. M. Keck Lab. of Hydraul. and Water Resources, California Institute of Technology, Pasadena, CA. 86 pp.

Chu, V. H. (1979). “L. N. Fan's data on buoyant jets in a crossflow.” J. Hydr. Div., ASCE, 105, 612–617

Davis, L.R., and M.A. Shirazi. 1978. A review of thermal plume modeling. Keynote address. pp. 109-126. In: Proceedings of the Sixth International Heat Transfer Conf., Amer. Soc. Mech. Eng., August 7-11, 1978, Toronto, Canada.

Davis, L.R. 1998. Fundamentals of Environmental Discharge Modeling. Ist Edition E-book. https://doi.org/10.1201/9780203755310

Doneker, R. L., and G. H. Jirka (1990), "Expert System for Hydrodynamic Mixing Zone Analysisof Conventional and Toxic Submerged Single Port Discharges (CORMIX1)," Report No. 109 EPA/600/3-90/012, U.S. Environmental Protection Agency, Env. Research Laboratory, Athens, Georgia.

Ecology 2018. Appendices: Permit Writers Mannual. Water Quality Program. Washington State Department of Ecology. WAC

Fan, L. N. (1967). “Turbulent buoyant jets into stratified or flowing ambient fluids.”Rep. No. KH-R-15, Calif. Inst. of Technol., Pasadena, California.

Fischer, E. J. List, R. C. Y. Koh, J. Imberoer and N. H. Brooks. 1979 Mixing in Inland and Coastal Waters. Academic Press, 1979. 483 pp.

Fofonoff, N.P., 1985. Physical properties of seawater: a new salinity scale and equation of state for seawater. J. Geophys. Res. 90, 3332. https://doi.org/10.1029/JC090iC02p03332

Frick, W.E., 1984. Non-empirical closure of the plume equations. Atmos. Environ. 18, 653–662. https://doi.org/10.1016/0004-6981(84) 90252. https://doi.org/10.1016/0004-6981(84)90252-X

Frick, W.E., Baumgartner, D.J., Fox, C.G., 1995. Improved prediction of bending plumes. J. Hydraul. Res. 32, 935–950. https://doi.org/10.1080/00221689409498699

Frick, W.E. 2004. Visual Plumes mixing zone modeling software. Environmental Modelling & Software 19 (2004) 645–654.

Fischer, H.B., List, E.J., Koh, R.C.Y., Imberger, J., Brooks, N.H., 1979. Mixing in inland and coastal waters.

Academic Press, New York, USA

Fofonoff, N.P., 2008. Physical properties of seawater: a new salinity scale and equation ofstate for seawater. J. Geophys. Res. 90, 3332. https://doi.org/10.1029/jc090ic02p03332.

Jirka, G.H., and P. J. Akar (1990), "CORMIX2: Expert System for Multiport Diffuser Discharges," Proc. Nat'l. Conference on Hyd. Eng., ASCE, San Diego, California

Jirka, G. and S.W. Hinton, 1992. User's guide for the Cornell mixing zone expert system (CORMIX). National Council of the Paper Industry for Air and Stream Improvement, Inc.. Technical Bulletin No. 624. February, 1992.

Jones G.R., Nash J.D., Jirka G.H. 1996. CORMIX3: an expert system for mixing zone analysis and prediction of buoyant surface discharges, DeFrees Hydraulics Laboratory, Cornell University (1996)

Kannberg, L.D., and L.R. Davis. 1976. AA experimental/analytical investigation of deep submerged multiple buoyant jets. EPA-600/3-76-101. U.S. Environmental Protection Agency, Corvallis, OR. 266 pp.

Koh, R.C.Y., and L.N. Fan. 1970. Mathematical models for the prediction of temperature distributions resulting from the discharge of heated water in large bodies of water. Water Pollution Control Research Series Rep. 16130DW0101/70. U.S. Environmental Protection Agency, Corvallis, OR. 219 pp.

Lee, J.H.W., Cheung, V., 1991. Generalized Lagrangian model for buoyant jets in current. J. Hydraul. Eng. 116, 1085–1106.

Liseth, P. 1976. Wastewater Disposal by Sub merged Manifolds. Jour. Hydraul Div.,. Proc. Amer. Soc. Civil Engr., 102, 1.

Liseth, P., 1970. Mixing of merging buoyant jets in stagnant receiving water of uniform density. Ph.D. Thesis, University of California, Berkeley.

Mancini, J., 1978. Numerical estimates of coliform mortality rates under various conditions. Journal of Water Pollution Control Federation. November 1978.

Morton, B. R., Taylor, G., Turner, J. S. 1956. Turbulent Gravitational Convection from Maintained and Instantaneous Sources. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, Volume 234, Issue 1196, pp. 1-23

Muellenhoff, W.P., A.M. Soldate, Jr., D.J. Baumgartner, M.D. Schuldt, L.R. Davis, and W.E. Frick. 1985. INITIAL MIXING CHARACTERISTICS OF MUNICIPAL OCEAN DISCHARGES VOLUME I - PROCEDURES AND APPLICATIONS

Pearson, E.A. 1956. An Investigation of the. Efficacy of Submarine Outfall Disposal of. Sewage and Sludge. Pub No. 14. State Water Pollution Control Board, Sacramento, CA. 258 pp.

Premathilake L, T Khangaonkar. 2019. FVCOM-plume – A three-dimensional Lagrangian outfall plume dilution and transport model for dynamic tidal environments: Model development. Marine Pollution Bulletin, 149: 110554. https://doi.org/10.1016/j.marpolbul.2019.110554

Priestly, C.H.B, and F.K. Ball. 1955. Continuous convection from an isolated source of heat. 81 (1955), pp. 144-157.

Roberts, P.J.W. 1977. Dispersion of buoyant waste discharge from outfalldiffusers of finite length. Rep. No. KH-R-35. W. M. Keck Lab. of Hydraul. and Water Resources, California Institute of Technology, Pasadena, CA. 183 pp.

Roberts, P.J.W. 1979a. Line plume and ocean outfall dispersion. J. Hydraulic. Div., Am. Soc. Civ. Eng. 105:313-331.

Roberts, P.J.W. 1979b. A mathematical model of initial dilution for deepwater ocean outfalls. Proceedings of a specialty conference on conservation and utilization of water and energy resources. San Francisco, CA. Aug. 8-11. Am. Soc. Civ. Eng. pp. 218-225.

Roberts, P.J.W. 1983. Mixing and transport. J. Water Pollut. Control Fed. Literature Review Issue 55:752-57.

Roberts, P.J.W. 1984. Mixing and transport. J. Water Pollut. Control Fed. Literature Review Issue 56:692-697.

Roberts, P.J.W. 1985. Mixing and transport. J. Water Pollut. Control Fed. Literature Review Issue 57:634-638.

Roberts, P.J.W., W.H. Snyder, and D.J. Baumgartner, 1989 a. Ocean outfalls I: submerged wastefield formation. ASCE Journal of Hydraulic Engineering. 115. No. 1. pp 1-25.

Roberts, P.J.W., W.H. Snyder, and D.J. Baumgartner, 1989 b. Ocean outfalls II: spatial evolution of submerged wastefield. ASCE Journal of Hydraulic Engineering. 115. No. 1. pp 26-48.

Roberts, P.J.W., W.H. Snyder, and D.J. Baumgartner, 1989 c. Ocean outfalls III: effect of diffuser design on submerged wastefield. ASCE Journal of the Hydraulic Engineering. 115. No. 1. pp 49-70.

Roberts, P.J.W., 1990. Outfall design considerations. In: Le Mehaute, B., Hanes, D.M. (Eds.), The Sea, Ocean Enginereing Sciences. John Wiley & Sons, Ltd, New York, USA, pp. 661–689.

Rouse, H., C.S. Yih, H.W. Humphreys. Gravitational convection from a boundary source. Tellus, 4 (1952), p. 201

Sotil , C. A. 1971. Computer program for slot buoyant jets into stratified ambient environments. Tech. Memo 71-2. W. M. Keck lab. of Hydraul. and Water Resources, California Institute of Technology, Pasadena, CA. 21 pp.

U.S. EPA. 1982. Modifications of secondary treatment requirements for discharges into marine waters. Federal Register, November 26, 1982. 47(228):53666-53685. Washington, DC.

U.S. EPA, 1985. Rates Constants and Kinetics Formulations in Surface Water Quality Modeling. EPA Environmental Research Laboratory, Athens, GA. EPA/600/3-85/040

U.S. EPA. 1991. Technical Support Document for Water Quality Based Toxics Control. EPA/505/2-90-001.

U.S. EPA 1994. Amended Section 301(h) Technical Support Document. EPA 842-B-94-007. September 1994. Office of Water.

Wright, S.J. Mean Behavior of Buoyant Jets in a Crossflow. J. Hydraul. Div. 1977, 103, 12944

Appendix – A : PLUMES2.0 Model Validation and Testing

Verification and testing were conducted for the three main stages of the PLUMES2.0 development process. The objective was to ensure that the Fortran based PLUMES2.0 reproduced the Visual Plumes UM3 model outputs for both near-field and far-field calculations. The first stage of testing and verification was conducted after the completion of near-field development. A comprehensive set of scenario cases were simulated with PLUMES2.0 covering a wide range of ambient currents, stratifications (temperature and salinity), discharge flowrates, and several diffuser configurations (i.e., single port/multiport/different port orientation angles/staggered/non-staggered). The results were then compared with the corresponding outputs produced by UM3. In the second stage of testing, similar comprehensive scenarios were examined for the far-field plume parameters computed with Brooks principles implemented in PLUMES2.0. The model results were compared against the Brooks far-field parameters produced by Visual Plumes. Third stage testing and verification was conducted to ensure the proper operation of the GUI.

A.1 Near-field dilution

The model testing and validation were conducted for three major plume parameters: (1) Plume diameter; (2) Plume height; and (3) Plume dilution at termination of near-field mixing. Figures A.1, A.2, and A.3 compare PLUMES2.0 model performance against UM3 results. As shown in the figures, the PLUMES2.0 produces almost identical results to those from UM3 for all the cases. Although we expect the results to be identical, the differences are caused by differences in precision levels in language specific intrinsic mathematical functions. Table A.1 shows the model skill metric (Average absolute relative error percentage) for each plume parameter which is less than 0.5%. This demonstrates that the PLUMES2.0 can robustly reproduce the UM3 model performance for the near-field plume parameters together with the fate of the plume (trapping, surfacing, merging, and bottom contact).

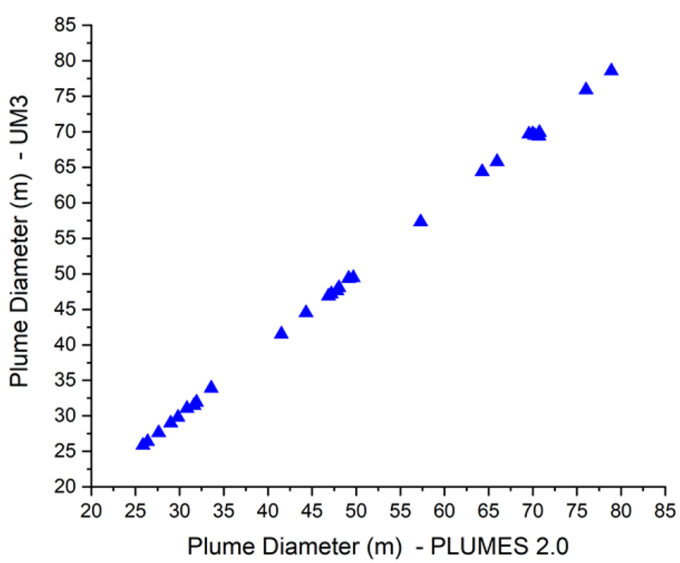


Figure A.1: The Comparisons of PLUME 2.0 results and UM3 model results; Plume diameter.

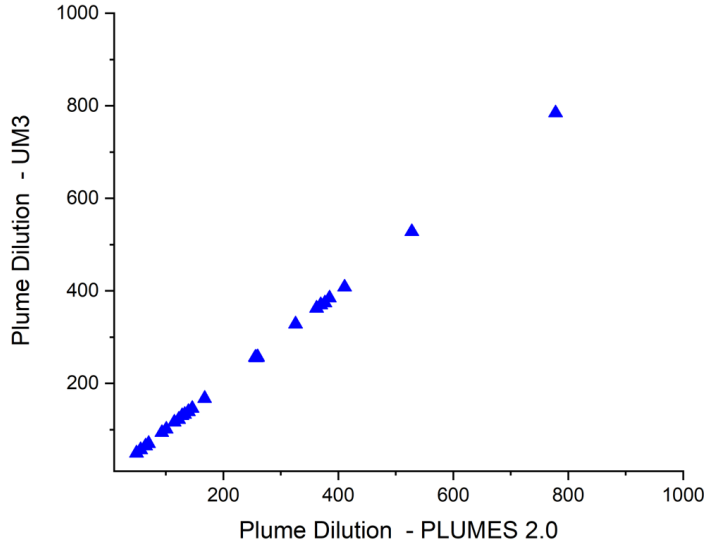


Figure A.2: The Comparisons of PLUME 2.0 results and UM3 model results; Plume Dilution.

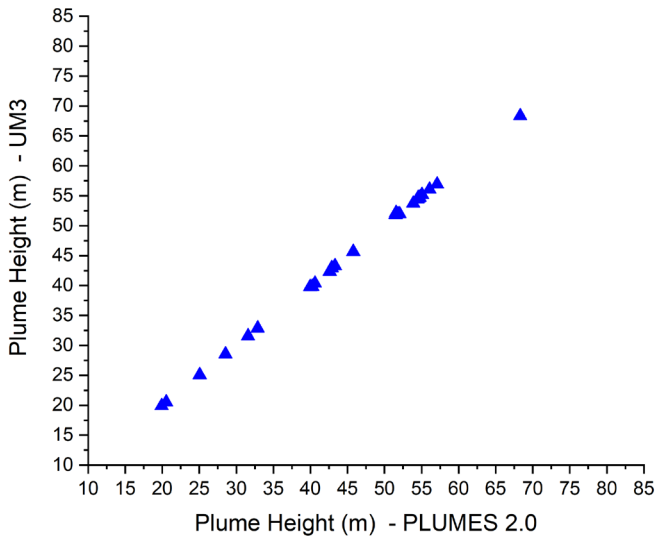


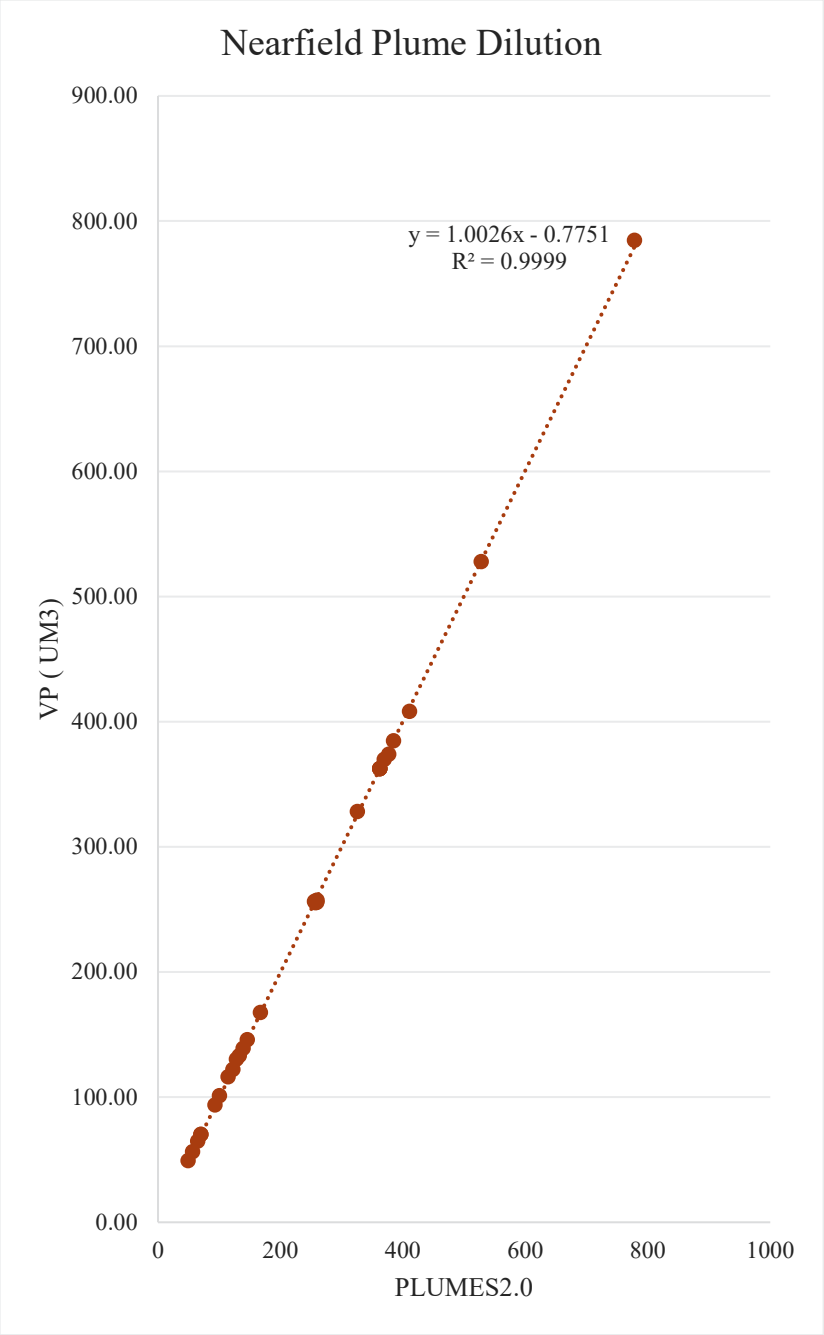
Figure A.3: Comparison of PLUMES2.0 results and UM3 model results; Plume height at the conclusion of initial dilution.

Table A.1: PLUMES2.0 model skill relative to Visual Plumes for near-field plume parameters

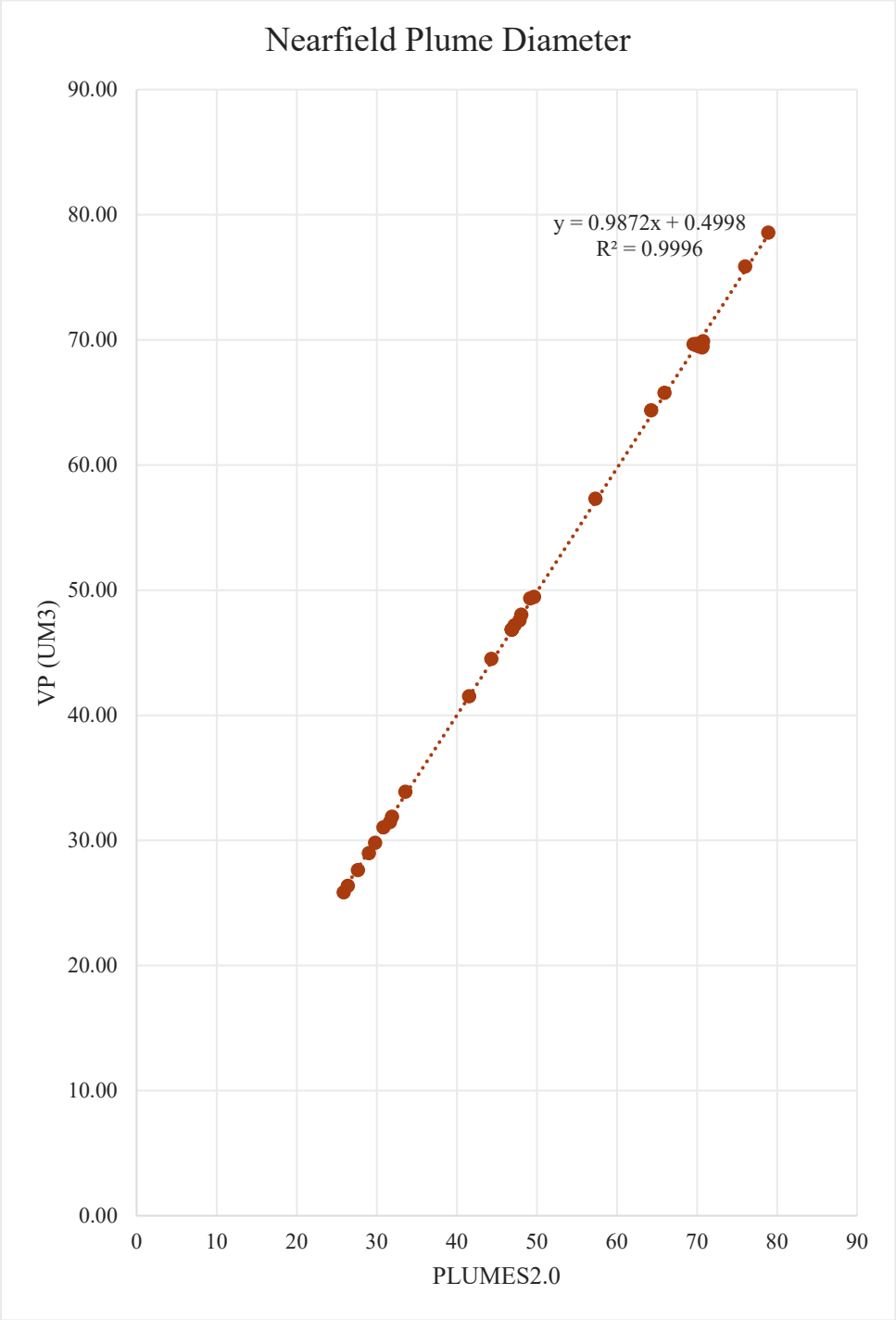
Model Skill Assessment – Averaged absolute error percentages		
Plume diameter (%)	Plume height (%)	Plume dilution (%)
0.37	0.26	0.41

R^2 statistics for plume dilution was calculated as $R^2 = 0.9999$. Similarly, for plume diameter, $R^2 = 0.9996$. Both of these meet the acceptance criteria of $R^2=1.0$.

Nearfield Plume Dilution	
PLUMES2.0	VP (UM3)
132.714803	133.00
362.409223	362.40
122.412558	122.00
114.73999	116.10
128.264756	130.20
527.947369	527.90
325.749201	328.20
376.840461	373.90
369.656583	369.70
384.58932	384.60
410.996562	408.10
362.409203	362.40
362.409206	362.40
362.409211	362.40
167.45121	167.50
145.845113	145.80
778.153221	784.50
255.734072	256.20
259.15555	255.60
259.356519	256.00
259.649461	257.40
256.902562	256.20
257.164794	255.30
93.0727418	93.69
139.245838	138.80
100.646919	101.10
64.7438084	64.74
56.3660052	56.37
70.0746303	70.07
70.073837	70.07
49.0750747	49.08



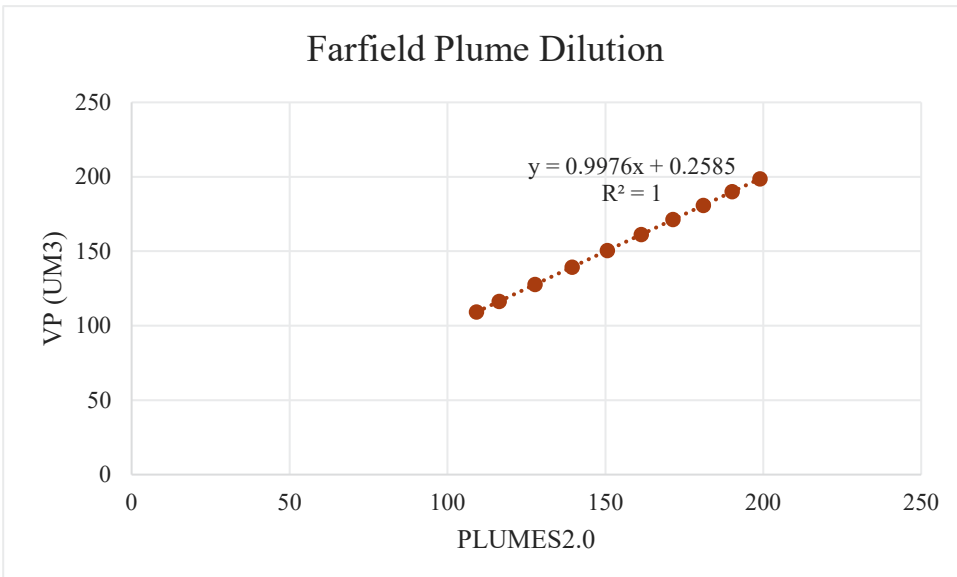
Nearfield Plume Diameter	
PLUMES2.0	VP (UM3)
65.9576239	65.79
46.8691099	46.87
31.6317789	31.48
30.8299141	31.06
33.5800443	33.90
57.3057271	57.31
44.3267589	44.51
47.8163873	47.61
47.1856959	47.19
48.0446643	48.04
49.6646848	49.47
46.8681112	46.87
46.8682562	46.87
46.8684768	46.87
31.9081993	31.91
29.811709	29.81
49.147933	49.36
69.5674545	69.68
70.6634704	69.40
70.6760233	69.47
70.7648909	69.90
69.976245	69.70
70.2115447	69.50
64.2614455	64.39
78.8906576	78.59
76.0334049	75.89
41.5216712	41.52
27.6311397	27.63
26.3766259	26.38
25.8573627	25.86
29.0015315	29.00



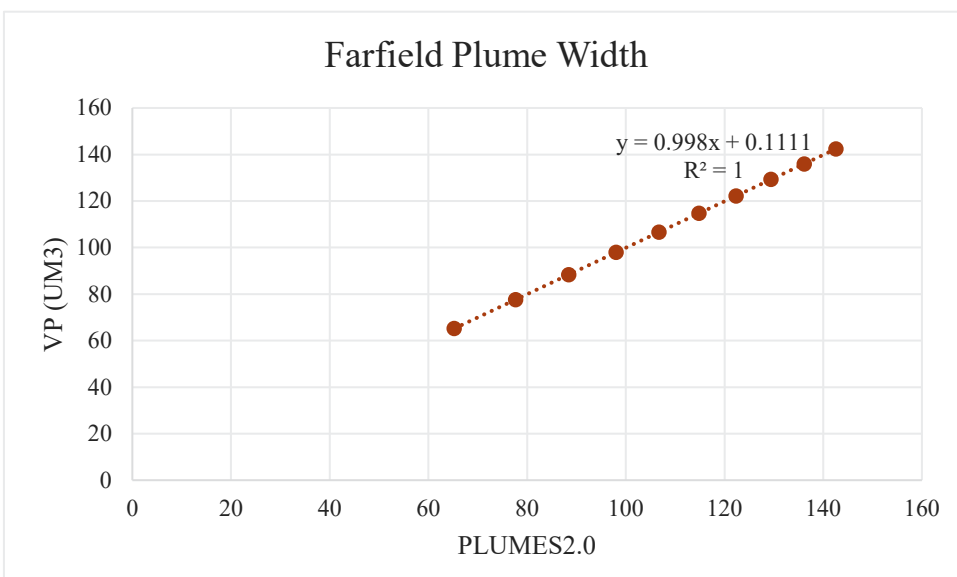
A.2 Far-field dilution

Since the Brooks far-field model is comprised of a set of explicit analytical equations, no specific numerical modeling technique is required to calculate the associated far-field parameters. PLUMES2.0's far-field results were compared against the Visual Plumes model results for various far-field ambient conditions as part of quality assurance and quality control validation. The model comparisons shown in Figure A.4 is for 12 cases of different ambient conditions with both constant eddy diffusivity and 4/3 power law-based eddy diffusivity (option 1 and 3). The relative error percentages for dilution of plume width predictions of PLUMES2.0 in comparison with Visual Plumes for 12 far-field cases are listed in Table A.2. For each test, $R^2 = 1.0000$, which meets the evaluation criteria of $R^2 = 1.0$.

Farfield Plume Dilution	
PLUMES2.0	VP (UM3)
109.182	109.2
116.41	116.4
127.797	127.7
139.479	139.4
150.703	150.6
161.35	161.2
171.445	171.3
181.04	180.9
190.191	190
198.947	198.7



Farfield Plume Width	
PLUMES2.0	VP (UM3)
65.217	65.19
77.715	77.66
88.464	88.39
98.042	97.95
106.764	106.7
114.825	114.7
122.356	122.2
129.45	129.3
136.175	136
142.583	142.4



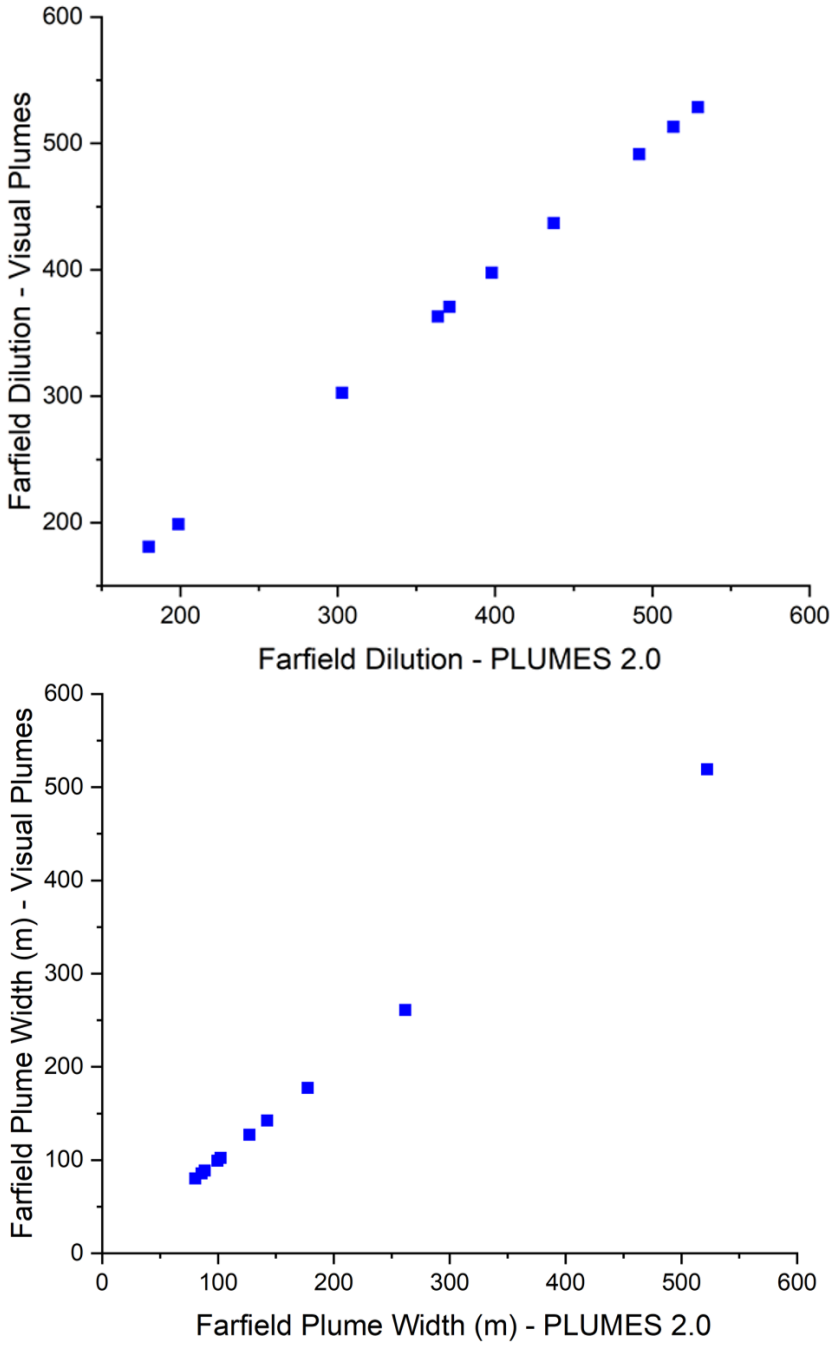


Figure A.4: Comparison of PLUMES2.0 far-field prediction with Visual Plume results – Far-field dilution and plume width.

Table A.2: PLUMES2.0 model skill relative to Visual Plumes for far-field plume parameters for the 12 test cases

Dilution Ratio Relative Error (%)	**Plume Width** Relative Error (%)
0.12	0.13
0.25	0.26
0.06	0.09
0.13	0.15
0.06	0.07
0.09	0.10
0.54	0.07
0.07	0.62
0.03	0.06
0.06	0.08
0.12	0.13
0.25	0.26

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