Numerical Study on Dynamical Structures and the Destratification of Vertical Turbulent Jets in Stratified Environment

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Abstract: The law of pollutant emission and diffusion in stratified waters is a common issue. In this paper, numerical study on the interaction between vertical turbulent jets and the pycnocline is carried out to study the problems of jet’s emission through the large eddy simulation (LES). A trigonometric function disturbance (TFD) method is developed to ensure the velocity distribution of the jet in the horizontal plane yield to Gaussian profile. Numerical simulations are carried out in the range of $1.11 < Fr_p < 4.77$, corresponding to $1393 < Re_p < 5979$, where the Froude number $Fr_p$ and the Reynolds number $Re_p$ are defined at the entrance of pycnocline. The coherent structure and internal waves are observed at the pycnocline during the process of jets impinging. After the impingement, the destratification effects can be found. It can be found that $Fr_p = 3$ is a threshold value for the interaction between jets and the pycnocline. When $Fr_p > 3$, the interaction becomes intensely. Furthermore, the fitting formula of the radial momentum flux dissipation rate that is used to describe the decay of energy contained by the jets during the impinging process, is established through the dimensionless analysis. As a result, the influence range of the jet on the horizontal plane can be evaluated by $Re_p$. It is also found that the destratification of jets is mainly affected by the velocity of the internal wave induced by jets. In addition, by employing the dimensionless time $T$ related to that velocity, the law of destratification varies with dimensionless time is obtained, which can be summarized as follows: Due to the influence of the first internal wave, the thickness of the pycnocline increases rapidly and reaches a critical value at $T = 1.4$, after that, the increase of the thickness of the pycnocline becomes linear.

Keywords: jet; pycnocline; interface structure; large eddy simulation (LES)

1. Introduction

The pollutant emission and diffusion in water environment is a common issue and these problems, such as the leakage of wastewater [1] and oil [2], can be generalized as the problems of jets [3]. In addition, the jet is also one of the motivations that cause the movement of fluid near jet’s trajectory, which may lead to the changes of water environment. For example, particles would be resuspended [4] with the influence of jets, which causes the changes of sedimentation in reservoirs and lakes [5]. As a result, there are many studies concerning properties of the jet in unstratified water. On the other hand, pycnocline can be commonly found in oceans, estuaries and lakes, normally produced by salinity or seasonal temperature stratification. The existence of stratification has many adverse effects on the water environment, such as substantial hypolimnetic oxygen depletion, which has a negative impact on aquatic systems and water quality [6]. Therefore, in stratified lakes and reservoirs with weak
hydrodynamics, artificial destratification measures are often used to control stratification [7–10], mainly including underwater aeration [11] and mechanical disturbance [12]. However, the destratification of jets has not attracted people’s attention yet. Furthermore, the properties of jets in stratified water are quietly different from that in unstratified environment. Camassa [13] claimed that the rising height of the jet was affected by the density gradient, and it could not penetrate through the pycnocline if the momentum of the jet is not large enough. That is to say, the development of jets would be restricted by the pycnocline. So, it is necessary to study the interaction between jets and the pycnocline and it will provide reference for studying the emission law of pollutant and the destratification of jets.

Many studies indicated that the properties of jets in unstratified environment could be indicated by the values of some dimensionless parameters [14–16]. Turner [14] defined the initial density Froude number \( Fr_0 = u_0 / \sqrt{r_0 g'_0} \), where the subscript ‘0’ refers to values at the source; \( u_0 \) is the vertical velocity of the jet; \( r_0 \) is the radius of the nozzle; \( g'_0 \) is the reduced gravity), and studied the rise height of negatively buoyant fountains in the range of \( 0.55 < Fr_0 < 11.8 \). The result indicated that the fountain stopped at the initial maximum rise height \( z_m \) due to the negative buoyance. Then, the fountain fell back down around the up-flowing fountain core and settled at a steady-state height \( z_s \), and the rise height ratio \( \lambda = z_m / z_s \approx 1.43 \). Burridge [15,16] studied the negatively buoyant fountain in the range of \( 0.4 < Fr_0 < 45 \) and presented that the range of \( \lambda \) was \( 0.5~2.0 \). Furthermore, the negatively buoyant jet was divided into four classes: very weak, weak, intermediate, and forced.

With reference to dimensionless parameters of jets in unstratified water, researchers also defined some parameters to study jets in the stratified environment. Ezhova [17] defined the Froude number before the jet reaching the pycnocline \( Fr_t = 0.5 U_{max} / \sqrt{R_t g''} \), where \( U_{max} \) and \( R_t \) are the maximum velocity and the radius of the jet at the entrance to the thermocline, and studied the penetration height of jets under stratified environment in the range of \( 0.6 < Fr_t < 1.89 \) by both experimental and numerical simulation. Druzhinin [18] defined the Froude number of the jet as \( Fr = w_0 / N_0 D_0 \), (where \( w_0 \) is the initial velocity of the jet; \( D_0 \) is the nozzle diameter of the vertical jet; \( N_0 = g \Delta \rho / \rho_0 D_0 \) is the buoyancy frequency at the center of the pycnocline; \( \rho_0 \) is the density at the center of the pycnocline; \( \Delta \rho \) is the density difference between upper and lower layers) and studied the interaction between jets and the pycnocline by DNS.

The interaction between jets and the pycnocline is studied based on the parameters mentioned above. During the rising process, the density of the jet at the pycnocline entrance is equal to the density of lower layer due to the jet entrains the surrounding fluid [17]. After the jet penetrates the pycnocline, the momentum of the core of upward flow rapidly decays due to negative buoyancy when the jet penetrates through the pycnocline. Then the jet falls back and impinges on the pycnocline after reaching the maximum penetration height. As a result, internal waves are generated at the pycnocline [19–22]. Figure 1 is the schematic diagram. Ezhova [19–21] compared the theoretical results based on the conservation of energy with the LES results and indicated that the theoretical penetration height was related to \( Fr_t^2 \), but the penetration height was overestimated at the largest \( Fr_t \) because turbulence during the entrainment was not taken into account. Coté [22] analyzed the entrainment and the coherent structure after the jet penetrated into the upper layer. It was found that with the effect of the shear force caused by the counterflow of the jet, vortices with opposite directions were formed in pair on both sides of the pycnocline. Druzhinin [18] indicated that the jet maintained a stable state after breaking through the pycnocline when the Froude number was less than 2. However, when the Froude number was greater than 2, the jet began to oscillate, which would be accompanied by the generation of internal waves.
The phenomenon of the jet penetrating the pycnocline is similar to the scheme of the bubble plume that is usually applied to destratification. Mcdougall [23] first put forward the double plume model of bubble plume in a stratified environment. Kim [24] studied the relationship between bubble size, diffusing area, and de-stratification efficiency through physical experiments. Destratification of a single-phase buoyant jet is similar to bubble plume. Neto [25] compared bubble plume with single-phase plume and indicated that bubble plume also generated a fountain at the pycnocline. In addition, the height of fountain and entrainment properties of the bubble plume were also similar to the single-phase plume, and the generation of internal waves could be seen from the experimental results. Therefore, it is necessary to research the destratification of single-phase jet.

In this study, a three-dimensional (3D) LES model is established to study the interaction between vertical jets and the pycnocline and the destratification effects of jets. The research is carried out with the following three aspects: (1) Analyzing the impingement process and coherent structure of the jet under stratified environment; (2) obtaining hydraulic properties of interaction between jets and a pycnocline; (3) developing destratification function of jets. In Section 2, the numerical models together with the TFD method are introduced. In Section 3, verifications and parameters of the model are introduced. In Section 4, the simulation results are discussed. The results of this study can provide theoretical basis for hydraulic and entrainment properties during the emission of pollutants in the stratified environment.

2. Governing Equations and Numerical Methods

2.1. Model Description

As shown in Figure 2, a 3D numerical model is established to study hydraulic properties of the interaction between a vertical jet and a pycnocline. The size of water tank is $1 \, \text{m} \times 1 \, \text{m} \times 0.5 \, \text{m}$ in $x$, $y$ and $z$ direction respectively. The non-uniform grid system is adopted to save computation costs. As shown in Figure 3, the whole computational domain is discretized into $100 \times 100 \times 80$ nodes, and the time step is 0.001 s corresponding to the grid scale. Due to the inaccuracy in simulating the round nozzle with rectangular grid, a rectangular nozzle is adopted instead, which is also used by Chen [26]. The nozzle (width $L_0 = 0.88 \, \text{cm}$) is located at the center of the bottom in the stratified environment. The velocity of jets in our cases is in the range of $0.2 \, \text{m/s}$ to $1.0 \, \text{m/s}$. The pycnocline is located at $z = 0.25 \, \text{m}$. $\rho_u$ and $\rho_d$ are the density of upper and lower layers, respectively. $h_u$ and $h_d$ are the height of the upper and lower layers, respectively. The density of the jet is the same as that of the lower layer.
The dimensionless nozzle size is 0.0088 that is calculated by the width of nozzle and the horizontal size of the computational domain. There are many references about the horizontal dimensionless nozzle size both in numerical simulations and experiments. Table 1 shows the comparison of the dimensionless nozzle size between previous researches and this study. It can be found that the dimensionless nozzle size is suitable in this paper.

**Table 1. Dimensionless nozzle size of previous researches compared with the size in this study.**

| Dimensionless Nozzle Size | Stratified/Unstratified | Experimental/Numerical | $Fr_0$ | $Re_0$ | Reference |
|---------------------------|-------------------------|------------------------|--------|--------|-----------|
| 0.025                     | Stratified              | Numerical              | 7–22   | -      | Ezhova [17]|
| 0.01                      | Stratified              | Experimental           | -      | 896–1066| Ansong [27]|
| 0.017                     | Stratified              | Experimental           | -      | 6900 and 12,400| Cotel [22]|
| 0.0083                    | Stratified              | Experimental           | 9–18.8 | 2979–5960| Ahmad [3]  |
| 0.0041–0.0088             | Unstratified            | Experimental           | 0.3–40 | 563–4037| Burridge [16]|
| 0.033                     | Stratified              | Numerical              | 1–9    | -      | Druzhinin [18]|
| 0.0088                    | Stratified              | Numerical              | 8.36–27.89 | 1760–8800| This study |
2.2. Governing Equations

The 3D, unsteady, incompressible, filtered continuity and Navier–Stokes equations (NSEs) with the Boussinesq approximation in rectangular coordinates are written as:

Continuity equation:
\[
\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (1)
\]

Momentum equations:
\[
\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho_a} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \bar{u}_i}{\partial x_j} - \tau_{ij} \right) + \left( \frac{\rho}{\rho_a} \right) g_i \quad (2)
\]

Scalar transport equation:
\[
\frac{\partial c}{\partial t} + \frac{\partial (\bar{u}_j c)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\alpha + \alpha_t) \frac{\partial c}{\partial x_j} \right] \quad (3)
\]

where the subgrid Reynolds stresses \( \tau_{ij} = -2\nu_t S_{ij} = -\nu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \), the turbulent viscosity coefficient \( \nu_t = (C_s \Delta)^2 \sqrt{2S_{ij}S_{ij}} \), the Smagorinsky coefficient \( Cs \) is taken as a constant in this study and \( Cs = 0.10 \), \( \Delta = (\Delta x \Delta y \Delta z)^{1/3} \), \( g_i \) is the gravitational acceleration; \( \rho_a \) is the density of the ambient water; the molecular diffusion coefficient \( \alpha = \nu \) and the turbulent diffusion coefficient \( \alpha_t = \nu_t \). In this study, the Prandtl Number (Pr) and the turbulent Prandtl Number (Pr_t) are set to 0.7 and 0.3, respectively.

The fluid density \( \rho \) is related to the scalar concentration, which can be given by:
\[
\rho = \rho_0 + \beta c \quad (4)
\]

where \( \rho_0 = 998 \text{ kg/m}^3 \) (pure water); \( \beta \) is the concentration contraction coefficient; and \( c \) is the concentration.

2.3. Numerical Methods and Boundary Conditions

An operator splitting method is used to solve the governing equations mentioned above. At each time step, the flow equations are split into three steps: advection, diffusion and pressure propagation steps, while the transport equation is split into two steps: advection and source steps. In this study, a combination of the Lax-Wendroff and the quadratic backward characteristic methods is employed to solve the flow advection. The central difference method is used to discretize the diffusion step. The projection method is used with the help of the continuity Equation (1) to solve the additional terms, including the pressure and the gravitational forces in the NSEs. A stable and robust conjugate gradient stabilized method (CGSTAB) is employed to solve the Poisson pressure equation. The details of the numerical method are to be found in Zhu’s [28] and Lin’s [29] study.

Zero gradient condition is adopted at the wall of the tank, and sponge boundary [30] with a thickness of 10 cm is imposed near the wall in order to reduce the influence of the wall. Rigid lid assumption is used on the free surface due to the jet is far enough from the surface. No slip boundary condition is adopted at the bottom of tank. Initial condition is a stable stratified water environment. The vertical velocity distribution of the jet is given by top-hat function:
\[
w_0(x) = -w_0 \left[ 1 - \left( \frac{x^2}{L_0^2} \right)^3 \right] \quad (5)
\]

where \( w_0 \) is the initial velocity of the jet; \( x \) is the coordinate defined by Figure 2; \( L_0 \) is the initial width of the jet.
It is necessary to add disturbance at the jet inlet boundary in order to simulate turbulence characteristics of jets. A trigonometric function disturbance (TFD) method is developed based on S. Menow’s [31] azimuthal forcing method. Compared with S. Menow’s azimuthal forcing method, a random angle $\theta_r$ and an extra cosine function are employed in the TFD method to ensure velocity distribution of the jet in the horizontal plane yield to Gaussian profile. The disturbance formulas are written as follows:

$$u = A_u w_0(r) \sum_{n=1}^{N} \sin(2\pi ft/n + \theta_r)$$

$$v = A_v w_0(r) \sum_{n=1}^{N} \cos(2\pi ft/n + \theta_r)$$

where $A_u$ and $A_v$ are the amplitudes of fluctuation in $x$ and $y$ direction, respectively; $\theta_r$ is the random angle varying from 0 to $\pi$ with time; $N$ is the number of modes (set to 6); $f$ is the frequency determined by the jet preferred mode corresponding to a Strouhal number. Strouhal number of the jet is roughly between 0.2 and 0.8, thus, in this study Strouhal number is set to 0.3.

Although employing the azimuthal forcing method can achieve ideal vertical velocity decay of jets by several scholars [32,33], the velocity distribution of the jet in the horizontal plane is difficult to yield to the Gaussian distribution. Because only sine function is used in azimuthal forcing method which causes the correlation between $u$ and $v$. After applying the TFD method, there is a difference with a period of $\pi/2$ in disturbances between the $x$ and $y$ directions. Therefore, it can be guaranteed that the $u$ and $v$ components of the jet velocity are uncorrelated. In order to compare the traditional azimuthal forcing method with the TFD method, the $u$ and $v$ at the plane of $Z = 20$ from the results simulated through two methods are extracted and a plot of the values of $u/w_c$ and $v/w_c$ is shown in Figure 4. It can be seen that the points obtained through the TFD method distribute randomly in the $uv$ plane, while the points obtained through the traditional azimuthal forcing method almost make up a line of $u = v$, namely the $u$ and $v$ are uncorrelated by employing the TFD method.

![Figure 4. The correlation between $u$ and $v$ at the plane of $Z = 20$.](image)

In addition, the comparisons between the results simulated via the azimuthal forcing method and the TFD method are shown in Figure 5. It can be observed that the profiles of vertical velocity and concentration simulated through the TFD method are better yield to Gaussian profile than that simulated through azimuthal forcing method. More validations can be found in Chapter 3.
is the velocity of the first internal wave produced by the jet; \( \rho \) is the density of the upper layer; \( \rho_0 \) is the density of the lower layer; \( \rho_\Delta \) is the density difference between upper and lower layers; \( c_{aw} \) is the velocity of the first internal wave produced by the jet; \( h_c \) is the critical pycnocline thickness; \( u, v, \) and \( w \) are velocity components in \( x, y, \) and \( z \) directions; \( h \) is the initial pycnocline thickness; \( r_{inf} \) is influence range of jets in horizontal direction; \( r_s \) is the radial distance from the observation point to the axis of jet, in this study \( r_s \) is set to 0.3 m.

Druzhinin [18] claimed that jet dynamics were governed by the values of the Froude Number and Reynolds number. Burridge’s [15] study indicated that the nozzle size and the velocity of the jet could be described through the dimensionless Froude Number and Reynolds number. Burridge's [15] study indicated that the nozzle size and the velocity of the jet could be described through the dimensionless Froude Number and Reynolds number. In order to extend our model to the real scale in the stratified environment, the Froude number and Reynolds number at the entrance of pycnocline, which are based on the characteristics of jets and the pycnocline, are defined as follow:

\[
R = \frac{r}{L_0}, \quad (X, Y, Z) = \frac{(x, y, z)}{L_0}, \quad (U, V, W) = \frac{(u, v, w)}{w_0}
\]

\[
H = h/L_0, \quad H_c = h_c/L_0, \quad p_i = p_i/L_0
\]

\[
P_s = p_s/L_0, \quad R_{inf} = r_{inf}/L_0, \quad T = c_{aw}t/r_s
\]

where \( L_0 \) is the width of the nozzle; \( u, v, \) and \( w \) are velocity components in \( x, y, \) and \( z \) directions; \( h \) is the initial pycnocline thickness; \( h_c \) is the critical pycnocline thickness; \( p_i \) is the initial penetration height of jets; \( p_s \) is the stable penetration height of jets; \( r_{inf} \) is influence range of jets in horizontal direction; \( c_{aw} \) is the velocity of the first internal wave produced by the jet; \( r_s \) is the radial distance from the observation point to the axis of jet, in this study \( r_s \) is set to 0.3 m.

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\[
Fr_p = \frac{0.5w_{cp}}{\sqrt{r_p g'}}
\]

\[
Re_p = \frac{w_{cp}r_p}{V}
\]

where \( g' = g_0 \rho / \rho_0 \) is one of the characteristics of the stratified water environment; \( \rho_0 \) is the density of the upper layer; \( \rho_0 \) is the density difference between upper and lower layers; \( w_{cp} \) is the velocity of jet axis at the entrance to the pycnocline; \( r_p \) is the half-width of jets at the entrance to the pycnocline. \( w_{cp} \) and \( r_p \) represent the properties of jet at the entrance of pycnocline.
In addition, the initial Froude number and Reynolds number of jets at the source is defined as:

$$Fr_0 = \frac{w_0}{\sqrt{L_0 g'}} \quad (11)$$

$$Re_0 = \frac{w_0 L_0}{v} \quad (12)$$

where $w_0$ is the initial vertical velocity of jets; $L_0$ is the width of the nozzle.

3. Model Validation

Numerical cases are detailed in Table 2. Cases A0 and A1 are used for validation. Cases A1~A9 are the jets with different momentums and same initial pycnocline thickness. These cases are used to study the hydraulic properties of the vertical turbulent jets interacting with the pycnocline. The velocities of jets in cases B1~B2 and B3~B4 are 0.5 m/s and 0.8 m/s, respectively. While the dimensionless initial thicknesses of the pycnocline in cases B1, B3 and B2, B4 are 2 and 4, respectively. Cases B1~B4 are used to study the destratification effects of jets.

Table 2. The parameters of different cases. The Froude number $Fr_p$ and Reynolds number $Re_p$ are defined at the entrance of the pycnocline, corresponding to the initial Froude number $Fr_0$ and Reynolds number $Re_0$. The details of values used in Table 2 can be found in Section 2.4.

| Cases | $w_0$ | $Fr_0$ | $Re_0$ | $Fr_p$ | $Re_p$ | $H$ | $\rho_a$ (kg/m$^3$) | $\rho_d$ (kg/m$^3$) |
|-------|-------|--------|--------|--------|--------|-----|---------------------|---------------------|
| A0    | 0.88  | 24.53  | 7744   | -      | -      | -   | 998                 | 998                 |
| A1    | 0.2   | 5.58   | 1760   | 1.11   | 1393.07| 1.0 | 998                 | 1033                |
| A2    | 0.3   | 8.36   | 2640   | 1.37   | 1723.63| 1.0 | 998                 | 1033                |
| A3    | 0.4   | 11.16  | 3520   | 2.26   | 2828.66| 1.0 | 998                 | 1033                |
| A4*   | 0.5   | 13.94  | 4400   | 2.83   | 3553.58| 1.0 | 998                 | 1033                |
| A5    | 0.6   | 16.74  | 5280   | 3.19   | 3993.69| 1.0 | 998                 | 1033                |
| A6    | 0.7   | 19.52  | 6160   | 3.66   | 4588.04| 1.0 | 998                 | 1033                |
| A7*   | 0.8   | 22.31  | 7040   | 4.07   | 5099.32| 1.0 | 998                 | 1033                |
| A8    | 0.9   | 25.10  | 7920   | 4.39   | 5500.41| 1.0 | 998                 | 1033                |
| A9    | 1.0   | 27.89  | 8800   | 4.77   | 5979.11| 1.0 | 998                 | 1033                |
| B1    | 0.5   | 13.94  | 4400   | 2.83   | 3553.58| 2.0 | 998                 | 1033                |
| B2    | 0.5   | 13.94  | 4400   | 2.83   | 3553.58| 4.0 | 998                 | 1033                |
| B3    | 0.8   | 22.31  | 7040   | 4.07   | 5099.32| 2.0 | 998                 | 1033                |
| B4    | 0.8   | 22.31  | 7040   | 4.07   | 5099.32| 4.0 | 998                 | 1033                |

* The parameters in B1~B2 and B3~B4 are refer to those in A4 and A7 respectively.

3.1. Mesh Refinement Study

To illustrate that the grid size used in this paper does not affect the calculation results, cases A0 and A9 are separately simulated by a coarse grid system ($80 \times 80 \times 60$) and a fine grid system ($150 \times 150 \times 110$). The comparisons between these two grid systems with medium grid system ($100 \times 100 \times 80$) which is adopted in the verification are shown in Figure 6. As shown in Figure 6a, the vertical velocities at the jet axis in three different grid systems have little differences. It proves that the medium grid size can accurately simulate the jet. As shown in Figure 6b, the vertical velocity profiles of jets at the pycnocline in fine and medium grid systems have little differences. It proves that the medium grid size can accurately simulate the interaction between jets and the pycnocline.
In our model, the courant (CFL) number in all three directions are controlled to be less than 1.0. The CFL number in X, Y, and Z directions are defined as follows:

\[
\text{CFL}_x = \Delta t \frac{u}{\Delta x}, \quad \text{CFL}_y = \Delta t \frac{v}{\Delta y}, \quad \text{CFL}_z = \Delta t \frac{w}{\Delta z}
\]  

(13)

The initial time step is set to 0.001 s in our model, and the maximal velocity is 1.0 m/s at the jet nozzle, and the minimum grid size is 0.0011 m at the jet nozzle. It can be estimated that the maximum CFL number is about 0.9 in our model. Furthermore, the dynamic time step method is used in our LES code to avoid CFL exceeding the threshold value, namely 1.0. If the CFL number is larger than 1.0, sub-steps (\(\Delta t\)) will be employed for computation automatically instead of the original time step \(\Delta t\). In addition, case A9 is chosen to analyze the CFL number. Figure 7 shows the mean CFL number varying with Z at the central line of the jet. It can be found that the CFL number is always less than 1.0.

3.2. Validation for the Turbulent Jet in a Unstratified Fluid

In order to validate the fully developed jet adopting the TFD method, a case (A0) of a turbulent jet in a homogeneous fluid is carried out and mean vertical velocity are compared with the result of Xu’s laboratory experiments [34]. The size of computational domain and the number of grids are described in Section 2.1. The initial velocity of the vertical jet at the bottom is 0.88 m/s, and the jet density is the same as the environment fluid. A numerical concentration contained by the jet is initially set as 10 mg/L to trace the jet trajectory, which actually, has no effects on the fluid density.

Figure 8 shows the comparison between numerical results and experimental results of Xu’s work. It can be seen that the decay of the axial vertical velocity of the jet in the LES is in good agreement with Xu’s experimental results.

Figure 6. Mesh refinement study. (a) Vertical velocity decay of the jet axis in Case A0. (b) Vertical velocity profiles of jets at the pycnocline in Case A9.

Figure 7. The courant (CFL) number varying with Z at the jet axis. (a) Instantaneous CFL. (b) Mean CFL.

Figure 8 shows the comparison between numerical results and experimental results of Xu’s work.
The profiles of the velocity and concentration of the jet in horizontal plane yield to the Gaussian distribution:

\[
\frac{w}{w_c} = \exp \left[ -\left( \frac{r}{b} \right)^2 \right] \tag{14}
\]

\[
\frac{c}{c_c} = \exp \left[ -\left( \frac{r}{b} \right)^2 \right] \tag{15}
\]

where \(w_c\) is the vertical velocity of jet axis; \(c_c\) is the concentration of jet axis, \(b\) is the half width of the jet.

Numerical concentration and velocity of \(Z = 10, Z = 20, Z = 30\) are extracted for verification. As can be seen from Figures 9 and 10, the velocity and the concentration distribution are close to Gaussian distribution.

Figure 8. Comparison between numerical results and experimental results.

Figure 9. Gaussian and simulated velocity profile of the jet on the horizontal plane.
Figure 10. Gaussian and simulated concentration profile of the jet on the horizontal plane.

3.3. Validation of the Jet in a Stratified Fluid

The laboratory experiment of a vertical jet in a stratified environment by Ezhova [21] is adopted to verify the development of the jet in the stratified environment in our model. The $Fr_p$ of case A1 is the same as that of the laboratory experiment; thus, case A1 is used to verify the vertical velocity profile of the jet at the pycnocline. Comparison of the result from the LES model ($Fr_p = 1.11$) with the vertical velocity at the thermocline from the experiment of Ezhova and Troitskaya is shown in Figure 11.

Figure 11. Comparison of present large eddy simulation (LES) data with vertical velocity profile of jet at the pycnocline by Ezhova and Troitskaya.

4. Results

4.1. The Process of Impingement

As shown in Figure 12, the process of the interaction between the jet and the pycnocline, and the generation of internal waves are illustrated by the instantaneous fields of density during $T = 0.24$–$0.67$ in case A3. When the jet penetrates into the upper layer at dimensionless time $T = 0.24$, a domelike structure is formed at the top of the jet. Meanwhile, the jet does not break up and there is no obvious vortex at the pycnocline. Then at $T = 0.27$, the vertical velocity at the top area of the jet decreases to 0.
due to the negative buoyance, but the core of the jet below the top area still retains some momentum and keep rising. Then at $T = 0.3$, part of the fluid falls back from the top of the jet, and core of the jet rises to its highest level before complete collapse. This level is defined as the initial penetration height $P_i$ in this study. When $T = 0.49$, the jet collapses, and the counterflow penetrates into the lower layer under the action of momentum, which causes a sag generated at the pycnocline around the jet. Meanwhile, the pycnocline around the jet becomes thick with the influence of turbulence. At $T = 0.58$, the pycnocline around the jet bounces back and internal waves generated during this process. According to the last contours of Figure 12 at $T = 0.67$, the pycnocline settles after the internal wave propagates far away. The pycnocline becomes thicker compared with that at $T = 0.24$–0.3. Subsequently, a fountain, which oscillates up and down around a certain level, is formed as a result of the interaction between the jet and the pycnocline. Thus, the mean penetration height is a constant value defined as stable penetration height $P_s$. The schematic of the comparison between the initial penetration height $P_i$ and the stable penetration height $P_s$ is shown in Figure 13, and the penetration height is further analyzed in Section 5.1.

![Figure 12](image_url)

Figure 12. Instantaneous density contours at the plane of $Y = 0$ during the jet impinging on the pycnocline in case A3. (a–f) corresponding to $T = 0.24$–0.67.
4.2. Generation of Coherent Structures.

The coherent structures caused by the interaction between the jet and the pycnocline directly affect the diffusion characteristic of the jet. These coherent structures are illustrated by the instantaneous fields of density at dimensionless $T = 0.6$, which are shown in Figure 14. The first observation is that the greater the $Fr_p$ is, the greater the degree of jets’ breaking up is after penetrating through the pycnocline. It can be also found that the greater the $Fr_p$ is, the higher the jets penetrate into the upper stratification layer. In addition, the counterflow is more evident with the increasing Froude number. As a result, more obvious internal waves are generated under the influence of the counterflow impinging on the pycnocline. If $Fr_p$ is small enough such as the case A1 ($Fr_p = 1.11$), the jet does not break up after penetrating through the pycnocline, and no internal waves are generated. In the case A3 with a greater $Fr_p$, although the jet breaks up after penetrating through the pycnocline and internal waves are generated, the turbulence is not strong and the amplitudes of internal waves are small. In the case A9 with the largest $Fr_p$, the jet flow has a more complicated structure, in the meanwhile, strong turbulence and internal waves with large amplitude are generated.

To quantify the coherent structures illustrated above, we calculate the turbulent kinetic energy $q = \sqrt{(u'^2 + v'^2 + w'^2)/3}$ of five observation points at $(\pm 2, 0, 26)$, $(0, \pm 2, 26)$, and $(0, 0, 26)$ after jets penetrate through the pycnocline. Figure 15 shows the sum of turbulent kinetic energy at five observation points in each case. According to the turbulent kinetic energy, we can divide the intensity of the interaction between the jet and the pycnocline into four classes. (1) No turbulence. When $Fr_p$ is small enough such as the case A1 ($Fr_p = 1.11$), the jet does not break up after penetrating through the pycnocline and the turbulent kinetic energy is close to 0. (2) Weak turbulence. Jets begin to break up after penetrating through the pycnocline. Such as cases A2–A4 where $Fr_p$ is in the range of 1.37 to 2.83. Linear regression is used to fit the increase of $q$ with the growth of $Fr_p$. The slope of the fitting line is only 0.015 and the turbulent kinetic energy maintains at about 0.1 which means that the increasing rate of $q$ is very slow in these cases. The reason for this phenomenon is that the turbulence caused by the interaction between jets and the pycnocline is not strong enough. (3) Intermediate. In cases A5 ($Fr_p = 3.19$) and A6 ($Fr_p = 3.66$), the change of turbulence energy experiences an obvious increase. (4) Intense turbulence. When $Fr_p$ is large enough, the jet completely breaks up due to the interaction with the pycnocline. Such as cases A7–A9 where $Fr_p$ is in the range of 4.07 to 4.77. The growth law of $q$ in this class is similar to Class 2. The slope of the fitting line is 0.014 and the turbulent kinetic energy maintains at about 0.2. It is because that the turbulence already reaches its most intense state, thus the turbulent kinetic energy can not increase any more.
From the streamlines in Figure 16a, it can be seen that the jet cannot penetrate through the pycnocline completely. Part of fluids penetrate through the pycnocline, and falls back to the pycnocline again. Hence, vortices are formed on the upper of the pycnocline by the shear force due to the horizontal flow. The other part which is blocked by the pycnocline also causes vortices formed under the pycnocline. As a result, vortices with opposite directions are formed in pair on both sides of the pycnocline, and the coherent structure is shown in Figure 16b.
4.3. Destratification of Jets

In order to illustrate the destratification of jets, the thicknesses of the pycnocline at about 60 s after impingement are extracted and the average of the dimensionless thicknesses ($\Delta H$) are calculated from $R = 15$ to $R = 35$. Figure 17a shows variations of $\Delta H$ with $Fr_p$ in cases A1~A9. According to Figure 17a, the thicknesses of pycnocline in all cases obviously increase with the influence of jets, which proves the destratification of the jet. It can be also found that the destratification effects have little differences when $Fr_p < 3$, however, the destratification effects obviously increase when $Fr_p > 3$. Figure 17b shows the distributions of the pycnocline thickness in cases A3, A6, and A9. The changes of $\Delta H$ are small between the different $R$, thus it is reasonable to use $\Delta H$ regardless of variation of $R$ to illustrate the destratification of jets. In addition, the destratification effect can be observed in a wide range around the jet.

5. Discussions

5.1. Quantitative Analysis of Hydraulic Properties of Jets Around the Pycnocline

The hydraulic properties near the jet impinging site at the pycnocline are discussed quantitatively in this section including the penetration height and momentum flux dissipation rate due to those properties directly affect the diffusion of jets around the pycnocline.

The initial penetration height $P_i$ and stable penetration height $P_s$ mentioned in Section 4.1 are defined referred to the penetration height of the buoyant jet in the unstratified environment. The later one has been well studied at present. The radial dynamical characteristic near the pycnocline is also different from that in an unstratified environment due to the influence of the interaction between jets and the pycnocline. In order to identify how far the jet can affects at the horizontal plane around

\[ \text{Figure 16. Instantaneous coherent structures of Case A6 at } T = 0.58. \text{ (a) Streamline around the jet at the plane of } Y = 0. \text{ (b) Isosurface of } \Omega = 0.55. \]

\[ \text{Figure 17. (a) Mean thicknesses of the pycnocline after the jet interaction with the pycnocline for 60 s.} \]

\[ \text{(b) The thickness distributions of the pycnocline in the range of } 15 < R < 35 \text{ in cases A3, A6, and A9.} \]
the pycnocline, the radius of the region where the radial velocity \((u_r)\) is greater than 1% of the initial velocity of the jet is defined as the horizontal influence radius \(R_{inf}\).

Figure 18a shows the relationship between dimensionless penetration height and \(Fr_p\). The results indicate that \(P_i\) increases linearly with the growth of \(Fr_p\) when \(Fr_p < 3\), and \(P_i/P_s\) is around 1.4 which is similar to the experimental results of Turner’s [14] and Hunt’s [15] studies, despite their studies in the unstratified fluid. When \(Fr_p > 3\), the value of \(P_i\) oscillates irregularly because the momentum of jets before impinging on the pycnocline is large, as a result, the collapse of jets occurs at different speeds after jets penetrate through the pycnocline. While \(P_s\) still increases linearly. Figure 18b shows the relationship between the dimensionless horizontal influence radius \(R_{inf}\) and \(Fr_p\). When \(Fr_p < 3\), the value of \(R_{inf}\) is very small and increasing slowly with the growth of \(Fr_p\). However, \(R_{inf}\) increases rapidly when \(Fr_p > 3\), in other words, the jet has a greater effect on the disturbance of the surrounding water at the pycnocline.

Both the results of initial penetration height and the horizontal influence radius indicate that \(Fr_p = 3\) is a threshold value, and that when \(Fr_p > 3\) the turbulence caused by the interaction between the jet and the pycnocline becomes larger. This turbulence also causes the dissipation of jets’ momentum. Using mean data to calculate the momentum flux dissipation rate \(K_d\) of the jet, the expressions are written as follows:

\[
K_d = 1 - \frac{FLh_{20}}{FL_{jet}} = 1 - \frac{\int_{Z_1}^{Z_2} 2\rho U_r U_r dz}{\int_0^{\infty} \rho U_r u_r dr}
\]

(16)

where \(FL_{h20}\) is the radial momentum flux at \(R = 20\) (where the pycnocline is not affected by the strong turbulence caused by the fountain). In this study, \(Z_1\) and \(Z_2\) are 15 and 35, respectively. \(FL_{jet}\) is vertical momentum flux of the jet at \(Z = 19\) (where the jet is not obviously affected by the pycnocline); \(U_l\) is the velocity; \(Ur\) is the radial velocity of the jet.

Figure 19 shows the relationship between \(K_d\) and \(Fr_p\). It shows that \(K_d\) increases with the growth of \(Fr_p\) before \(Fr_p\) reaches 3. After \(Fr_p = 3\), \(K_d\) becomes stable around 0.9. It claims that the turbulence becomes strong after \(Fr_p = 3\), therefore, the momentum of jets decay rapidly. The mentioned results further prove that \(Fr_p = 3\) is a threshold value for the interaction between jets and the pycnocline.
where the Reynolds number at the entrance of pycnocline in this study is defined as $Re_A$.

The exponential function is used to fit the calculation results of $A4$ to $A9$, and the regression formula is:

$$K_h = -0.19 + 1.25e^{-250.88 \frac{R}{Re_p}}, \quad 3500 < Re_p < 6000$$  \hspace{1cm} (17)

where the Reynolds number at the entrance of pycnocline in this study is defined as $Re_p = \frac{\omega_{cp}R_p}{v}$, and it is detailed in Section 3.

5.2. Quantitative Analysis of the Destratification of Jets

As illustrated in Section 4.1, pycnocline becomes thick with the influence of internal waves generated by the jet. Furthermore, the growth of pycnocline thickness $H$ with the variation of time is analyzed in this section. In order to link the destratification with internal waves generated by jets, the time $t$ is standardized by employing velocity of the first internal wave generated by the jet during the impingement. The definition of the dimensionless time $T$ is detailed in Section 2.4.
Only cases A3–A9 are chosen to study the destratification effect of jets, as there are no obvious internal waves in cases A1 and A2. Furthermore, the destratification effects of jets with different initial pycnocline thickness are studied through cases B1–B4. The average thickness of four points \((X = \pm 30, Y = 0; X = 0, Y = \pm 30)\) is measured as the thickness of pycnocline at \(R = 30\).

Figure 21 shows the relationship between the thickness of the pycnocline at \(R = 30\) and the dimensionless time \(T\). The change processes of the thickness can be divided into two stages. The first stage is \(T < 1.4\). The pycnocline is stable when jets are far away from the pycnocline. When \(T = 1\), the first internal wave reaches \(R = 30\), and the thickness of the pycnocline begins to increase obviously with the influence of internal waves. Then \((T = 1.4)\), the thickness of the pycnocline approaches to a certain value with the effect of the first internal wave. We define this value as the critical thickness \(H_c\), and the critical thickness in different cases are very close. Even in the cases with the largest initial pycnocline thickness, \(H_c\) is a little bit thicker than the cases with small initial pycnocline thickness.

The second stage is \(T > 1.4\), the increasing rate of the thickness slows down, and the process tends to be linear. The reason is that the influence of internal waves on the thickness of the pycnocline becomes smaller when the pycnocline thickness is larger than critical value. The relationship between the \(H\) and \(T\) in the range of \(1.4 < T < 6\) is fitted only through cases A3–A9 while cases B1–B4 in which the \(T\) only ends at 4 are used for further testing. The fitting formula is shown as follows:

\[
H = 1.06T + 3.27
\]

where \(H = h/L_0\) is the dimensionless thickness and \(T = c_\omega t/r_g\) is the dimensionless time as defined in Section 2.4.

![Figure 21. Dimensionless change in the thickness of the pycnocline varies with time for Cases A3–A9 (\(Fr_p = 2.26–4.77\)) and B1–B2 (\(Fr_p = 2.83\)) and B3–B4 (\(Fr_p = 4.07\)). The red solid line is the fitting line when \(T > 1.4\).](image)

Nash–Sutcliffe efficiency coefficient (donated as \(E_{ns}\) below), which is widely used to evaluate the performance of hydrological model, is employed to evaluate the performance of the fitting line Equation (18) in different \(Fr_p\). The definition of \(E_{ns}\) is shown as follows:

\[
E_{ns} = 1 - \frac{\sum_{i=1}^{n}(S_i - F_i)^2}{\sum_{i=1}^{n}(S_i - \bar{S})^2}
\]

where \(S_i\) is simulated value; \(F_i\) is fitted value; \(\bar{S}\) is the average of simulated values. The result of \(E_{ns}\) varying with \(Fr_p\) is shown in Figure 22.
This is why the thickness remains increasing when the thickness apparently slows down when the thickness of the pycnocline reaches the critical value. This is the reason that the increasing rate of the pycnocline thickness has a sudden increase at around $T = 1.1$, and this state can be sustained until $T = 1.4$. Above all, it could be concluded that the destratification effect is weaker when the thickness of the pycnocline reaches the critical value.

Figure 22. Nash–Sutcliffe efficiency coefficients of Cases A3–A9 ($Fr_p = 2.26$–$4.77$) and B1–B2 ($Fr_p = 2.83$) and B3–B4 ($Fr_p = 4.07$).

It can be found that $E_{ns}$ in all cases are larger than 0.5, which represents the good performance of the fitting line [36], despite that the results of B1–B4 are not used for fitting. Thus, the fitting formula can be extended to the cases with different initial pycnocline thicknesses. However, $E_{ns}$ is relatively small in the cases with the largest initial pycnocline thickness (Cases B2 and B4). In addition, in the cases with large $Fr_p$, such as A8 and A9, $E_{ns}$ decreases with the growth of $Fr_p$ because the destratification effects of A8 and A9, as shown in Figure 21, are much greater than that of the cases with a smaller $Fr_p$.

In order to find the reason that causes the change in the process of the thickness of pycnocline in Figure 21, the vorticity in $y$ direction is calculated as $\omega_y = \frac{\partial u}{\partial x} - \frac{\partial w}{\partial z}$. The instantaneous contour of $\omega_y$ at the plane of $Y = 0$ in case A6 is shown as Figure 23. Figure 23a is plotted at the time when the first internal wave arrives at $R = 30$. Moreover, the vorticity contour in $T = 2.2$ when the pycnocline thickness is larger than the critical value is shown in Figure 23b. In Figure 23a, the vorticity in the pycnocline is large; thus, the thickness of the pycnocline has a sudden increase at around $T = 1.1$, and this state can be sustained until $T = 1.4$. However, the vorticity in the pycnocline becomes obviously smaller after the thickness of the pycnocline reaches the critical value. This is the reason that the increasing rate of the thickness apparently slows down when $T > 1.4$. Moreover, there are still some vortices at the pycnocline, and this is why the thickness remains increasing when $T > 1.4$. Above all, it could be concluded that the destratification effect is weaker when the thickness of the pycnocline reaches the critical value.

Figure 23. Instantaneous contour of $\omega_y$ at $T = 1.1$ (a) and $T = 2.2$ (b) of case A6.
6. Conclusions

In order to study the law of pollutant emission and diffusion in stratified waters, the LES method with the TFD method on inlet boundary of jets is used to study the hydraulic properties of vertical turbulent jets interacting with a pycnocline and the destratification effects of jets. The conclusions are listed as follows.

1. The TFD method on inlet boundary of jets is developed to simulate the 3D turbulent jet, and the results of vertical velocity decay and horizontal velocity distribution are in good agreements with experimental data.

2. In terms of the degree of jets’ breaking up and the turbulent kinetic energy of the cases in this study, the intensity of the interaction between the jet and the pycnocline can be divided into four classes: No turbulence, weak turbulence, intermediate and intense turbulence.

3. According to the flow field, it can be concluded that the jet can’t penetrate through the pycnocline completely in the range of $1.11 < F_{rp} < 4.77$. One part penetrates through the pycnocline, and falls back to the pycnocline again. The other part is blocked by the pycnocline. As a result, vortices with opposite directions are formed in pair on both sides of the pycnocline.

4. $F_{rp} = 3$ is a threshold value of the interaction between jets and the pycnocline. When $F_{rp} > 3$, the interaction becomes intensely. Hence, the jet affects a wider range under the influence of the strong turbulence, and the momentum of the jet is dissipated more efficiently, with a greater destratification effect of jets. In addition, the fitting formula of the radial momentum flux dissipation rate is established through dimensionless analysis.

5. It is found that the destratification of the jet is mainly affected by the velocity of the internal waves produced by the jet. Regardless of the value of initial pycnocline thickness or $F_{rp}$, the pycnocline thickness reaches the critical value at $T = 1.4$ with the influence of the first internal wave. When $T > 1.4$, the increasing rate apparently slows down and the pycnocline thickness increases linearly in all cases due to the vorticity in the pycnocline becomes small obviously after the thickness of the pycnocline reaches the critical value.

Additionally, re-suspension and entrainment of particles can be caused by jets, which is a common feature and is a complex problem in stratified environments. The study in this paper would give a potential factor of re-suspension and entrainment of particles caused by jets.

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