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# 1 Large eddy simulations of 45° inclined dense 2 jets

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## 10 **Abstract:**

11 Submerged inclined dense jets (negatively buoyant jets) occur in many  
12 engineering applications such as brine discharges from seawater desalination  
13 plants and de-cooling water discharges from liquefied natural gas (LNG) plants,  
14 and their mixing behavior needs to be examined in details for the environmental  
15 impact analysis. In the present study, a detailed numerical investigation was  
16 performed using the Large Eddy Simulation (LES) approach with both the  
17 Smagorinsky and Dynamic Smagorinsky sub-grid scale (SGS) models to simulate  
18 the characteristics of the inclined dense jet with 45° inclination. The numerical  
19 predictions included the jet trajectory, geometrical characteristics, jet spread and  
20 eddy structures. Experimental measurements were also obtained for the validation  
21 of the LES predictions, and data from existing studies in the literature were  
22 included for comparison. Overall, the LES predictions were able to reproduce the  
23 geometric characteristics of the inclined dense jet in a satisfactory manner in most  
24 aspects. The dilution was however generally underestimated, which was attributed  
25 primarily to the inability of the SGS models to reproduce the convective mixing  
26 induced by the buoyancy-induced instability using the adopted grid spacing in the  
27 bottom half of the inclined dense jet.

28 *Keywords: Large eddy simulations; Brine discharges; Negatively buoyant jets;*  
29 *Buoyancy-induced instability*

30

# 1 **1 Introductions**

2 Effluents that have a density heavier than the ambient environment are often  
3 discharged directly into coastal waters using submerged outfalls, and the effluent  
4 discharges thus behave as dense jets. Typical examples include brine discharges  
5 from desalination plants and de-cooling water discharges from liquefied natural  
6 gas (LNG) plants. These effluent discharges can have an adverse influence on the  
7 local waterborne ecosystem [1,2]. In order to mitigate the potential environmental  
8 impact, it is essential to design the outfall in an optimal manner to achieve a rapid  
9 mixing of the brine effluent with the ambient waters. Hence, a good prediction of  
10 the outfall performance is important for design.

11         A submerged inclined outfall configuration is typically adopted for brine  
12 discharges in coastal waters, as the inclined dense jet exhibits a longer curvilinear  
13 trajectory before impacting the sea bed and hence the configuration can achieve a  
14 higher dilution. Figure 1 illustrates the schematic side view of the inclined dense  
15 jet in stagnant ambient, where  $z_t$  is the terminal rise height,  $x_r$  is the return point  
16 location,  $x_m$  and  $z_m$  are the horizontal and vertical locations of the centerline peak,  
17 respectively. Upon discharging from the bottom, the inclined dense jet first rises  
18 due to the initial momentum. After reaching the peak height, it then falls and  
19 impacts onto the seabed due to the negative buoyancy.

20         Many analytical and experimental studies had been conducted on inclined  
21 dense jets. Zeitoun et al. [3] performed a pioneering experimental study with  
22 various inclinations, and suggested an inclination of  $60^\circ$  (relative to the  
23 horizontal) to achieve the maximum dilution. The  $60^\circ$  inclination was then  
24 investigated in many subsequent experimental investigations [4-6], where both the  
25 jet geometrical and dilution characteristics were determined. Pincince and List [4]  
26 compared their experimental results with integral modelling predictions, and  
27 concluded that the integral model was able to predict the flow trajectories with  
28 reasonable accuracy while significantly underestimated the dilution. More  
29 recently, several studies [7-9] extended the investigations of negatively buoyant  
30 discharges to smaller inclinations of  $30^\circ$  and  $45^\circ$ , which are more feasible for  
31 outfalls in coastal regions where the near-shore bathymetry is relatively shallow.  
32 Their studies characterized the jet geometrical features, including the maximum

1 rise height and the impact/return point distances, as well as the dilution  
2 characteristics. Generally, these earlier analytical and experimental investigations  
3 indicated a dependence of the mixing characteristics with the discharge  
4 densimetric Froude number, which is defined as:

$$5 \quad Fr = \frac{U_0}{\sqrt{\frac{\rho_b - \rho_a}{\rho_a} gD}}$$

6 where  $U_0$  is the jet exit velocity,  $\rho_a$  and  $\rho_b$  are ambient and brine densities,  
7 respectively,  $g$  is the gravitational acceleration,  $D$  is the diameter of the discharge  
8 nozzle.

9 Numerical studies on negatively buoyant jets had also been performed in  
10 recent years. These studies mostly focused on vertical fountains [10-12]. The  
11 fountain is inherently different from the inclined dense jet because it re-entrains  
12 the negatively buoyant fluid which falls back around the vertical discharge.  
13 Vafeiadou et al. [13] was the first to report a numerical study on inclined dense  
14 jets. They employed the software CFX with the Reynolds Averaged Navier Stokes  
15 (RANS) approach and  $k-\varepsilon$  turbulence closure for the simulations. Oliver et al. [14]  
16 conducted a more detailed numerical investigation also using the RANS approach  
17 with  $k-\varepsilon$  turbulence closure. They compared their numerical results with those  
18 obtained from previous integral models and experimental observations, and  
19 concluded that the  $k-\varepsilon$  predictions provided a more accurate representation of the  
20 mixing processes compared to the integral models. More recently, Palomar et al.  
21 [15] reported an overview of the performances of some widely-used integral  
22 models, including CORMIX, VISUAL PLUMES and VISJET, on the analysis of  
23 inclined dense jets. Their study revealed significant discrepancies in the dilution  
24 predictions by these integral models for brine discharge modeling.

25 In the present study, we employ the Large Eddy Simulation (LES)  
26 approach to simulate the submerged inclined dense jet with a  $45^\circ$  inclination. LES  
27 is anticipated to provide a better prediction of the mixing behavior due to  
28 improved accuracy in resolving the large coherent eddies than the RANS  
29 approach. The objective is to evaluate the performance of LES on the predictions  
30 of both the kinematic and mixing behavior of the inclined dense jet in the near

1 field. Experimental measurements are also performed for the validation of the  
 2 LES predictions. In the following, we shall first introduce the computational  
 3 methodology. The numerical and experimental results are then presented and  
 4 compared to the available data in the literature.

## 5 **2 Computational Methodology**

### 6 **2.1 Governing equations**

7 In the LES approach, eddies are filtered into large and small sizes based on the  
 8 local grid spacing. Large eddies are then computed directly by solving the  
 9 instantaneous Navier-Stokes equations, while small eddies are modelled based on  
 10 assumptions such as the Boussinesq hypothesis. The filtered continuity,  
 11 momentum and concentration transport equations in Cartesian coordinates for  
 12 LES are as follows [16]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0 \quad (1)$$

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_j} + \bar{\rho} g_i + \frac{\partial^2}{\partial x_j^2} (\mu \tilde{u}_i) - \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

$$\frac{\partial (\bar{\rho} \tilde{\phi})}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{\phi} \tilde{u}_j) = \frac{\partial^2}{\partial x_j^2} (\Gamma \tilde{\phi}) - \frac{\partial Q_j}{\partial x_j} \quad (3)$$

13 where  $u_i, u_j$  are the velocity in  $i, j$  direction, respectively;  $\rho$  is the fluid density,  
 14  $p$  is the pressure,  $t$  is the time,  $g$  is the gravity acceleration,  $\mu$  is the fluid  
 15 viscosity,  $\Gamma$  is the scalar diffusivity,  $\phi$  is the scalar concentration; the overbar  
 16 indicates time averaged variables and the tilde indicates spatially filtered  
 17 variables;  $\tau_{ij} = \overline{\rho u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_j$  are the SGS Reynolds stresses and  
 18  $Q_j = \overline{\rho \phi u_j} - \bar{\rho} \tilde{\phi} \tilde{u}_j$  are the SGS scalar flux.

19 The effect of unresolved small scale eddies on the resolved flow can be  
 20 represented by a sub-grid scale (SGS) model. The Smagorinsky SGS model is  
 21 arguably the most commonly used among existing SGS models [17,18] and is also

1 adopted here. The SGS stress tensor and the SGS turbulent concentration flux in  
 2 the Smagorinsky model are modelled by

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\mu_t \tilde{S}_{ij} \quad (4)$$

$$Q_j = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{\phi}}{\partial x_j} \quad (5)$$

3 where  $\tau_{kk}$  is the isotropic part of SGS stress which usually can be neglected for  
 4 incompressible flows,  $Sc_t = 0.7$  [19,20] is the SGS turbulent Schmidt number

5 and  $\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$  is the rate of strain tensor for the resolved scale. The

6 remaining undetermined variable SGS eddy viscosity,  $\mu_t$ , is controlled by the  
 7 following equations involving  $\tilde{S}_{ij}$  proposed by Smagorinsky [21] and Lilly [22]:

$$\mu_t = \rho (C_s \Delta)^2 |\tilde{S}| \quad (6)$$

$$|\tilde{S}| = \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}} \quad (7)$$

8 where  $\Delta$  is the LES filter width which is defined by the grid spacing and  $C_s$  is  
 9 the Smagorinsky constant set to 0.17 herein.

10 Here, it should be noted that the coefficient  $C_s$  may not always be a  
 11 constant, and in fact can be better determined by a localized dynamic procedure  
 12 proposed by Germano et al. [23] and further modified by Lilly [24] as follow:

$$C_s^2 = \frac{\langle L_{ij} M_{ij} \rangle}{2 \langle M_{ij} M_{ij} \rangle} \quad (8)$$

$$L_{ij} = \widehat{\tilde{u}_i \tilde{u}_j} - \hat{\tilde{u}_i} \hat{\tilde{u}_j} \quad (9)$$

$$M_{ij} = \Delta^2 \left| \widehat{\tilde{S}} \right| \widehat{\tilde{S}_{ij}} - \hat{\Delta}^2 \left| \hat{\tilde{S}} \right| \hat{\tilde{S}_{ij}} \quad (10)$$

13 where the angular brackets indicate a spatial averaging procedure over directions  
 14 of statistical homogeneity, and the caret indicates a spatial filtered quantity on the

1 test-filter. This procedure can be further developed to include the scalar transport  
 2 as [24]

$$Sc_t = \frac{C_s^2}{C_\phi^2} \quad (11)$$

$$C_\phi^2 = \frac{\langle \varepsilon_j R_j \rangle}{\langle R_j R_j \rangle} \quad (12)$$

$$\varepsilon_j = \widetilde{\widetilde{u_j \phi}} - \widehat{\widehat{u_j \phi}} \quad (13)$$

$$R_j = \Delta^2 \left| \widetilde{\widetilde{S}} \right| \frac{\partial \widetilde{\widetilde{\phi}}}{\partial x_j} - \widehat{\widehat{\Delta^2}} \left| \widehat{\widehat{S}} \right| \frac{\partial \widehat{\widehat{\phi}}}{\partial x_j} \quad (14)$$

3 Equations (8) to (14) constitute what is now called the Dynamic Smagorinsky  
 4 SGS model.

5 In the present study, the equations were discretized using the finite volume  
 6 method and the simulations were performed with an open source code  
 7 OpenFOAM [25]. Specifically, the implementation in OpenFOAM was performed  
 8 with the turbulence solver twoLiquidMixingFoam and with both the Smagorinsky  
 9 and Dynamic Smagorinsky SGS models, respectively. The  
 10 twoLiquidMixingFoam is a solver for the mixture flow of two incompressible  
 11 fluids, and it has been used and validated in many studies [26,27].

## 12 **2.2 Flow configuration and computational setup**

13 The simulation domain was configured based on a fully submerged inclined jet  
 14 with an inclination of 45°. As shown in Figure 2, the origin of Cartesian  
 15 coordinates was set at the center of the discharge nozzle, the diameter of which  
 16 was  $D$ . The distances from the nozzle center to the back ( $L_b$ ), front ( $L_f$ ), left and  
 17 right sides ( $W$ ), surface ( $H_s$ ) and bottom ( $H_d$ ) boundaries were equal to or larger  
 18 than  $0.7DFr$ ,  $6DFr$ ,  $1.8DFr$ ,  $2DFr$ ,  $1DFr$ , respectively. Particular attention was  
 19 paid to the nozzle's cover water depth ( $H_s$ ) to avoid the surface contact of the  
 20 inclined dense jet [28]. In the present study, all the cases satisfied the criteria for  
 21 fully submerged 45° inclined dense jets ( $H_s > 1.6DFr$ ).

1           The computational domain was discretized with a stretched and structured  
2 mesh with increasing grid spacing from the center of the nozzle to the boundaries,  
3 as shown in Figure 3a. A double refinement was performed within a region that  
4 covered the core of the jet. The grids attached to the nozzle tube were generated  
5 by a tool of OpenFOAM, namely snappyHexMesh, which can divide a base cell  
6 into several sub-cells and then snap the sub-cell boundaries onto the surface of the  
7 nozzle tube, as shown in Figure 3b. The fluid viscosity and diffusivity were  $10^{-6}$   
8  $\text{kg}\cdot\text{m}^{-1}\text{s}^{-1}$  and  $10^{-9} \text{ m}^2/\text{s}$ , respectively. The other parameters for each case and their  
9 corresponding meshes are summarized in Table 1.

10           To examine the grid convergence, the method of Grid Convergence Index  
11 (GCI) [29] was used for the estimation of uncertainty in the CFD simulations.  
12 With GCI, the uncertainty is determined by a formula incorporating the results of  
13 two additional simulations of which a coarser mesh and a finer mesh are used  
14 individually. Figure 4 shows the dilution (represented in a line) and its uncertainty  
15 (represented in vertical bars) near the return point (at  $\sim 3.6FrD$ ) in Case S1.  $C$  and  
16  $C_0$  are the local and initial concentrations, respectively. From the figure, the  
17 uncertainty near the return point can be observed to be relatively small.

18           The boundary condition at the top surface was set to free slip, while a zero  
19 gradient open boundary was used for the other five outer boundaries. The nozzle  
20 surface was set as a velocity inlet with a uniform discharge velocity at a  
21 turbulence intensity of 10%. The corresponding dense fluid density was specified  
22 in Table 1. The other surfaces of the discharge tube were taken to be wall  
23 boundaries. A second order implicit backward scheme was used for the  
24 discretization of the temporal term. An upwind and a linear scheme were chosen  
25 to compute the divergence term and the Laplacian term, respectively. The  
26 convergence criterion of  $10^{-6}$  was set for the continuity, velocities as well as scalar  
27 concentrations. The time step interval was adjusted to ensure that the Courant  
28 number was less than 1.0. The computations were performed using parallel  
29 processors in the High Performance Computing centre of the Nanyang  
30 Technological University. As an example, for Case S2, the flow was computed up  
31 to 50 seconds, with a real-time computing duration exceeding 7 days with 4 nodes  
32 (each node having 16 cores).



## 1 **2.3 Experimental measurements**

2 In addition to the numerical simulations, the velocity and concentration  
3 distributions of the 45° inclined dense jet were also experimentally determined in  
4 the present study using the laser imaging techniques of Particle Image  
5 Velocimetry (PIV) and Planar Laser-Induced Fluorescence (PLIF), respectively.  
6 The experiments were performed in a glass test tank at the Nanyang  
7 Technological University, Singapore. The methodology and experimental setup  
8 adopted were very similar to those in Jiang et al. [28]. In the present experiments,  
9 the nozzle had an inner diameter of 5.8 mm, and the center of the nozzle was set at  
10 50 mm above the perspex bottom to avoid the influence of the bottom boundary.

## 11 **3 Results and Discussion**

12 In the following discussion, the LES predictions were compared with the  
13 experimental results obtained in the present study as well as previous  
14 experimental and numerical studies [7,8,14,30,15,31,32,9,33], including the jet  
15 trajectories, geometrical and dilution parameters, and turbulence characteristics.  
16 Except for the eddy structures shown in Figure 17, all the results were time-  
17 averaged over the period starting from 15 or 120 seconds (for simulation and  
18 experimental measurements, respectively), and lasting for approximately 60 to  
19 80 seconds.

20 Crowe [34] examined the possible influence of the bottom wall boundary  
21 in the mixing characteristics of the inclined dense jet. Based on his results, for the  
22 45° inclined dense jet, the minimum nozzle height ( $H_d$ ) necessary to avoid the  
23 boundary effect is  $\sim 0.6DFr$ . The previous studies with and without a bottom  
24 boundary were included for a comprehensive comparison herein, and the potential  
25 boundary effect has been clearly indicated for those with a bottom boundary.

### 26 **3.1 Jet trajectory and overall flow characteristics**

27 Figure 5 shows the mean velocity magnitude and normalized concentration  
28 contours ( $C/C_0$ ) of Case S1 at the centerline plane. From the velocity contours, the  
29 inclined dense jet first rises due to the initial discharge momentum until it reaches  
30 the peak height as shown in Figure 5. The concentration contours also show a

1 similar pattern. Subsequently, the negative buoyancy becomes dominant, and the  
2 inclined dense jet sinks downwards. The following jet characteristics, including  
3 the jet trajectory, geometrical and dilution characteristics, cross-sectional profiles  
4 and jet spread widths, can be obtained from the velocity magnitude and  
5 concentration contours at the center plane.

6 The jet centerline, also known as the trajectory, is a main geometrical feature of  
7 the inclined dense jet. The jet centerline can be defined as the locus of the  
8 maximum velocity or concentration at various cross sections from the respective  
9 velocity or concentration contour maps shown in Figure 5. Figure 6 presents the  
10 normalized jet concentration and velocity centerlines, with different  $Fr$  obtained  
11 from the LES predictions (with both Smagorinsky and Dynamic Smagorinsky  
12 models) and experimental measurements, where  $L_M = (\pi/4)^{1/4} DFr$  is the jet  
13 characteristic length scale. The experimental results from Kikkert et al. [8] and  
14 Oliver et al. [30] as well as the integral modelling predictions from Palomar et al.  
15 [15] are also included for comparison. From the figure, the normalized LES  
16 predictions with different  $Fr$  were similar to each other with slight divergences  
17 towards the downstream direction. The predictions with the Dynamic  
18 Smagorinsky model (D1) were almost identical to the Smagorinsky model (S1)  
19 for the jet trajectory. Compared with the present experimental results and those  
20 from previous studies, the LES predictions coincided with them near the nozzle  
21 and then diverged after the peak height, which was somewhat over-predicted.  
22 However, the divergence between the LES and experimental results was relatively  
23 smaller compared with the integral modeling predictions from Palomar et al. [15].  
24 It is noted that both the velocity (solid line) and concentration centerlines (dotted  
25 line) almost coincided with each other, which had also been noted in previous  
26 experimental studies [9]. In the following discussion, the centerline refers to the  
27 concentration centerline if not indicated otherwise.

### 28 **3.2 Geometrical and mixing features**

29 To assess the environmental impact of the brine discharge, the analysis must  
30 include the determination of the geometrical features of the inclined dense jet,  
31 including the terminal rise height, return point location as well as dilution at  
32 different locations. As discussed earlier, previous studies had verified that the

1 various normalized geometrical and mixing quantities of the inclined dense jet for  
2 a specific nozzle inclination are proportional to  $Fr$ . The various geometrical and  
3 mixing quantities predicted by LES are summarized in Table 2 together with the  
4 experimental results from the present and previous studies, with  $S_m$  and  $S_r$  being  
5 the dilution at the centerline peak height and return point, respectively.

6 In Table 2, the coefficients of the LES results are average values from the  
7 simulation runs shown in Table 1. The maximum variations of the coefficients  
8 from the Smagorinsky LES results are also indicated in the table. Based on the  
9 simulations, the variations were within around 10%, and most of them were  
10 approximately within 5%. The trend lines of the Smagorinsky LES results are also  
11 plotted for comparison based on these average coefficients in Figures 7-10.

12

### 13 *3.2.1 Terminal rise & centerline peak*

14 The terminal rise height,  $z_t$ , is crucial to the assessment of the environmental  
15 impact of the brine discharge. The criteria to determine the terminal rise height  
16 were different among the previous studies. Herein, the terminal rise height is  
17 defined as the peak height at the location where the concentration drops to 5% of  
18 the centerline peak concentration. This definition was also used in Jiang et al.  
19 [28]. Figure 7 presents the terminal rise height derived from the mean  
20 concentration fields at the centerline plane. The previous experimental and  
21 numerical results are included for comparison. It should be noted that the results  
22 of Oliver et al. [30] are represented by a trend line based on the averaged  
23 coefficient. From the figure, the LES predictions with the Smagorinsky and  
24 Dynamic Smagorinsky models coincided with each other, and they were close to  
25 the experimental results from Oliver et al. [30], Cipollina et al. [7], Kikkert et al.  
26 [8], et al.. The trend line based on the LES predictions (with the Smagorinsky  
27 SGS model) is plotted in the figure as well. The LES trend line was obviously  
28 closer to the experimental trend line from Oliver et al. [30] than the prediction of  
29 integral models presented by Palomar et al. [15].

30 Once the centerline was determined, the horizontal and vertical locations  
31 of the centerline peak,  $x_m$  and  $z_m$ , can be derived which are plotted against  $Fr$  in  
32 Figure 8. From the figure, it can be observed that the LES predictions agreed well

1 with the present experimental results as well as the results from previous studies.  
2 The normalized horizontal location  $x_m/D$  and vertical location  $z_m/D$  increased  
3 linearly with increasing  $Fr$ . The trend lines based on the averaged coefficients of  
4 the LES are also plotted in the respective figures. The scattering of the LES data  
5 points from the trend lines was relatively small, which demonstrated the  
6 consistency and accuracy of the predictions.

### 7 *3.2.2 Return point location*

8 Upon reaching the peak height, the inclined dense jet falls back onto the bottom  
9 due to its negative buoyancy. The location of the impact point, where the  
10 downward flow impinges onto the bottom, as well as the associated dilution is  
11 important parameters for the environmental impact analysis. The impact location  
12 can be dependent on the site conditions, including the source height and bed slope  
13 [35,36]. Here, the bottom effect was not considered, and the return point position  
14 (where the downward flow returns to the source height), is examined instead. The  
15 LES predictions were compared with corresponding experimental measurements  
16 from the literature.

17 Figure 9 shows the normalized horizontal location of the return point  
18 against  $Fr$ . The trend line based on the averaged LES coefficient is plotted in the  
19 figure as well. The differences between the two SGS models were small. It can be  
20 observed that the LES predictions were close to the experimental data especially  
21 from Kikkert et al. [8] but with slight over-predictions.

### 22 *3.2.3 Dilution*

23 The dilution at a specific location is defined as the initial concentration at the  
24 source over the local concentration,  $C_0/C$ . In the present study, the dilution at the  
25 return point is normalized and plotted against  $Fr$  in Figure 10. It can be observed  
26 that the results of previous studies deviated from each other, which may be due to  
27 their various bottom conditions as suggested by Oliver et al. [30]. Seen from the  
28 figure, the LES predictions were close to the results from Oliver et al. [30] but  
29 slightly lower. The LES averaged trend line based on the Smagorinsky results is  
30 also plotted in the figure. In comparison, the LES trend line still somewhat under-

1 predicted the experimental results, but the agreement was much better compared  
2 to the integral modeling predictions from Palomar et al. [15].

### 3 **3.3 Cross sectional profiles**

4 Figure 11 shows the normalized velocity and concentration profiles at different  
5 cross sections along the respective jet trajectories based on the Smagorinsky  
6 model. The cross sections began at  $s = 0.1FrD$ , where  $s$  is the distance from the  
7 nozzle center along the jet centerline, and the interval between the sections was  
8  $0.3FrD$ . As can be observed from the profiles, the flow pattern can be divided into  
9 the inner (or lower) and outer (or upper) halves in the regions below and above  
10 the trajectories of velocity or concentration maxima, respectively. Both the  
11 velocity and concentration profiles showed symmetry with respect to the  
12 centerline trajectory in the initial stage ( $s < 1.0FrD$ ). After  $s \approx 1.0FrD$ , asymmetry  
13 developed and the velocity or concentration profiles in the inner half were now  
14 wider than the outer half. Further downstream, the distributions became even  
15 more flattened.

16 In Figure 12, the non-dimensional cross-sectional profiles of the  
17 concentration  $C/C_c$  from Case S1 are plotted against  $r/b_c$ , where  $r$  is the radial  
18 distance (negative represents upper half),  $b_c$  is the concentration spread width and  
19  $C_c$  is the centerline concentration. A Gaussian profile is also plotted here for  
20 comparison. The results from previous studies are included by re-normalizing  $s/D$   
21 into  $s/FrD$ . In the near-nozzle region, the cross-sectional profiles obtained by LES  
22 showed self-similarity and distributed in the Gaussian manner. In the downstream  
23 region, the inner half began to deviate from the Gaussian profile, and the  
24 distortion increased with the distance from the nozzle within the range of the  
25 investigation in the present study. This phenomenon was also noted in previous  
26 experimental studies [8,9,33] and numerical study [14], which can be attributed to  
27 the additional spreading by the buoyancy induced instability.

### 28 **3.4 Jet spread**

29 In the present study, the jet spread widths are characterized based on the distance  
30 from the centerline to the 5% value of the centerline maximum. Figure 13 presents  
31 the velocity and concentration spread widths along the centerline trajectory. As

1 seen from the figure, the LES predictions were nearly identical between the  
2 Smagorinsky and Dynamic Smagorinsky models, and the spread widths of the  
3 LES predictions in the upper region were closer to the experimental data.  
4 However, the LES spread width was smaller in the inner region. Clearly, the  
5 enhanced inner spreading due to the buoyancy-induced instability was again not  
6 sufficiently captured by LES.

7         The variation of the jet spread width along the trajectory is further  
8 examined in Figure 14. In the figure, the upper and lower spread widths of the  
9 LES predictions with both the Smagorinsky and Dynamic Smagorinsky SGS  
10 models are extracted from Figure 13, and re-plotted against normalized  $s$ .  
11 Consistent with Figure 13, the differences between the Smagorinsky and Dynamic  
12 Smagorinsky models were small as shown in Figure 14a. Starting from the nozzle,  
13 the upper and lower spread widths of the LES predictions increased almost  
14 linearly in the beginning matching closely the experiment results, and then the  
15 rate of increase began to decline after  $s \approx 2.0FrD$  where the centerline peak was  
16 located. Around the peak region, the vertical momentum of the inclined dense jet  
17 became weak physically, while the buoyancy-induced instability at the bottom  
18 became prominent and drove the centerlines significantly lower, resulting wider  
19 spread widths in the experimental results. From the figure, the LES predictions  
20 were not able to fully capture this phenomenon due to the inadequacy of the SGS  
21 models with the adopted grid spacing. Subsequently, the spread widths resumed  
22 its increase at  $s \approx 2.7FrD$  in the downward plume region.

### 23 **3.5 Turbulence characteristics and eddy structures**

24 In Figure 15, the concentration turbulence intensity of the LES predictions at the  
25 centerline peak is computed and compared with the experimental data from Oliver  
26 et al. [30] and Papakonstantis et al. [32]. From the figure, the LES and  
27 experimental results showed similar distributions, having a peak value at  $r/b_c \approx -$   
28 0.7 in the outer region. Compared to Oliver et al. [30], LES under-predicted the  
29 turbulence intensity in the inner region where the buoyancy-induced momentum  
30 and instability were present.

31         The concentration turbulence intensity in the lateral direction was also  
32 extracted at the concentration peak and compared with the experimental data from

1 Papakonstantis et al. [32] and Lai and Lee [33]. It is noted, however, that both  
2 Papakonstantis et al. [32] and Lai and Lee [33] performed their experiments with  
3 the bottom boundary, while the present simulations were conducted without the  
4 boundary. The predictions of the Smagorinsky and Dynamic Smagorinsky models  
5 were comparably similar to the experimental data from Lai and Lee [34], but  
6 generally lower than Papakonstantis et al. [32], with twin peaks at  $r/b_c \approx \pm 0.5$ .

7 Figure 16 shows the concentration turbulence intensity at the return point.  
8 In Figure 16a, the azimuthal (normal to the jet centerline) distribution of the LES  
9 turbulence intensity is compared to Oliver et al. [30]. Similar to the centerline  
10 peak, the turbulence intensity at the return point also had a peak value at  $r/b_c \approx -$   
11 0.7. However, the turbulence intensity at the return point preserved the linear  
12 decline in the inner region. Compared to the experimental data, the LES  
13 predictions somewhat over-predicted the turbulence intensity. The lateral  
14 turbulence intensity at the return point is also plotted in Figure 16b. Unlike in  
15 Figure 15b, the turbulence intensity at the return point did not show the twin  
16 peaks in Figure 16b, and the Smagorinsky model predicted higher turbulence  
17 intensity in general.

18 The coherent structure of the inclined dense jet is important to the  
19 understanding the flow development, and can aid in the analysis of the mixing  
20 characteristics as well as the turbulence intensity. The LES eddy structures from  
21 Case S1, visualized by plotting the concentration contours in a diverging color  
22 map at the center plane, are compared with the present experimental PLIF images  
23 in a time sequence of 0.5s interval as shown in Figure 17. From the figure, the  
24 LES predictions had similar length scales to the experimental images in terms of  
25 the size of the coherent large eddies. Particularly, a series of similar-size vortex  
26 rings can be observed in the lower region below the centerline in the LES images.  
27 In contrast, the experimental images showed a fuller spectrum of large eddy sizes  
28 in the lower region. This discrepancy of the eddy sizes explained the lower  
29 turbulence intensity of the LES predictions in Figure 15, and also revealed the  
30 weakness of the SGS models with the adopted grid spacing in resolving the  
31 convective mixing by buoyancy-induced instability in the lower region.

## 1 **4 Conclusions**

2 In the present study, the 45° inclined dense jet was simulated numerically using  
3 LES with both the Smagorinsky and Dynamic Smagorinsky SGS models, and the  
4 simulation results were compared with the experimental measurements performed  
5 in the present study as well as from previous studies in the literature. The  
6 comparison covered the geometrical and dilution characteristics, the spread width  
7 characteristics and the eddy structures at the center plane.

8 In summary, both the standard Smagorinsky and the dynamic Smagorinsky  
9 LES predicted the geometrical characteristics reasonably well, including the  
10 return point location, horizontal and vertical location of the centerline peak, with a  
11 slight over-prediction of ~10% compared with the experimental data. Hence, the  
12 LES approach performed much better than the existing integral models in terms of  
13 the geometrical characteristics. LES is also much superior to the integral models  
14 in predicting the dilution at the return point. For dilution, the LES results had an  
15 under-prediction of ~20% compared with the experimental data, while the  
16 comparison with integral modeling results in Palomer et al. [15] yielded ~50%  
17 under-predictions. Note, however, that the recent improvements in integral  
18 modelling approach such as Reduced Buoyancy Flux (RBF) model from Oliver et  
19 al. [37] and Escaping Mass Approach (EMA) from Yannopoulos and Bloutsos  
20 [38] had achieved better results. In terms of the jet spread widths, the LES  
21 predictions were in reasonable agreement with the experimental measurements  
22 near the nozzle region, but beyond the centerline peak the under-prediction  
23 became prominent. The predicted turbulence intensity was satisfactory in the  
24 upper half but not the inner half. Together with the comparison of the eddy  
25 structures, it is obvious that, with the currently used mesh sizes, both the  
26 Smagorinsky and Dynamic Smagorinsky SGS models are not fully able to capture  
27 the convective turbulence under the influence of buoyancy. Improvement of the  
28 SGS model is therefore necessary in this direction, and it is being pursued in a  
29 further study.

30



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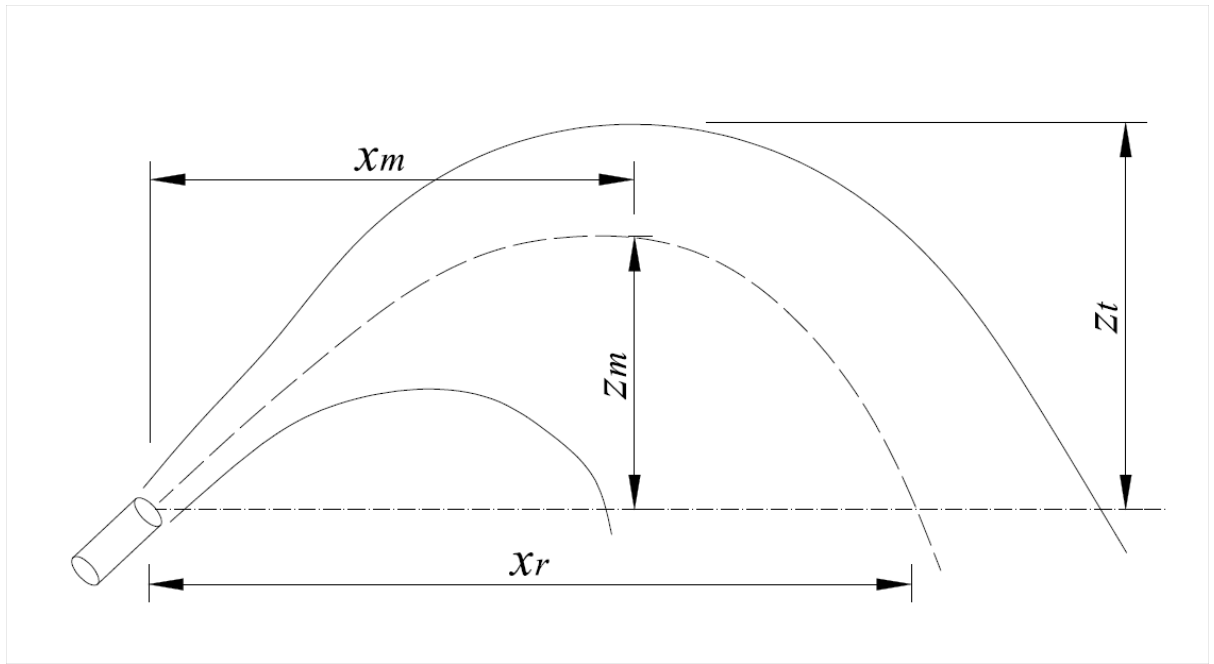
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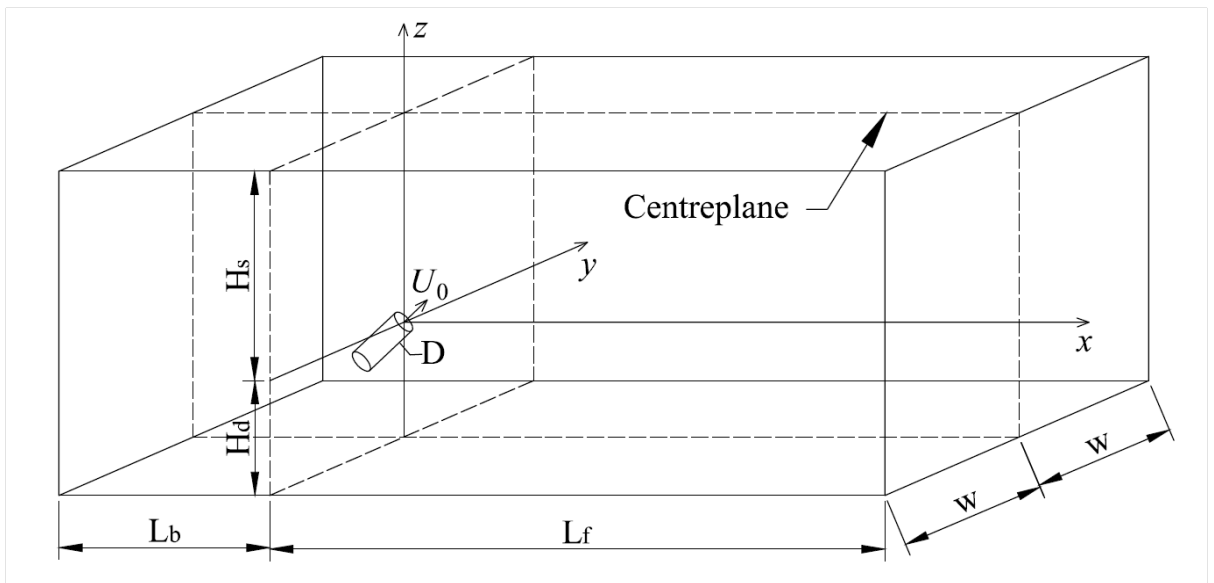
1 Figure 1 Schematic side view of an inclined negatively buoyant jet in stagnant  
2 ambient  
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4 Figure 2 Schematic diagram of the computational domain  
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6 Figure 3 (a) A structured mesh of the domain; (b) Detailed grids near the nozzle at  
7 the center plane  
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9 Figure 4 Dilution at the nozzle height level near the return point  
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11 Figure 5 Non-dimensional mean (a) velocity and (b) concentration contours at the  
12 center plane for Case S1  
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14 Figure 6 Comparison of normalized centerline trajectories  
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16 Figure 7 Comparison of normalized terminal rise height  
17  
18 Figure 8 Comparison of normalized centerline peak: (a) horizontal and (b) vertical  
19 locations  
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21 Figure 9 Comparison of normalized return point location  
22  
23 Figure 10 Comparison of normalized dilution at the return point  
24  
25 Figure 11 Cross-sectional profiles of (a) velocity and (b) concentration fields  
26 (Case S1)  
27  
28 Figure 12 Non-dimensional cross-sectional distributions of normalized  
29 concentration at (a)  $s/D_{Fr} = 0.5\sim 1.2$  and (b)  $s/D_{Fr} = 1.2\sim 2.5$   
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31 Figure 13 Comparison of the jet velocity and concentration spread widths  
32

1	Figure 14 Variation of (a) upper and (b) lower jet spread widths along the
2	trajectory
3	
4	Figure 15 Concentration turbulence intensity at the centerline peak in the (a)
5	vertical and (b) lateral directions
6	
7	Figure 16 Concentration turbulence intensity at the return point in the (a)
8	azimuthal and (b) lateral directions
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10	Figure 17 Eddy structures at the central plane: (Left) experimental images; (Right)
11	LES predictions (Case S1)
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17	Table 1 Parameters and mesh sizes
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19	Table 2 Comparison of coefficients
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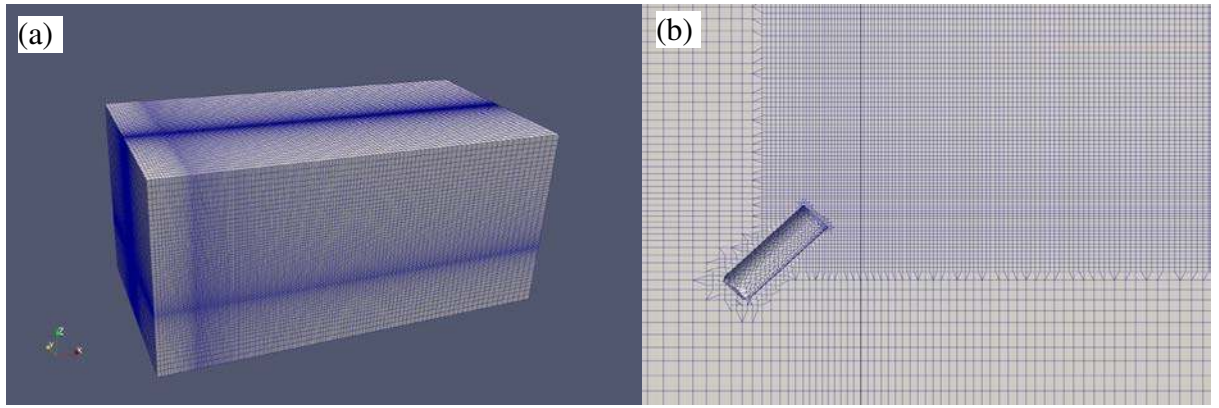
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Figure 1 Schematic side view of an inclined negatively buoyant jet in stagnant ambient



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Figure 2 Schematic diagram of the computational domain

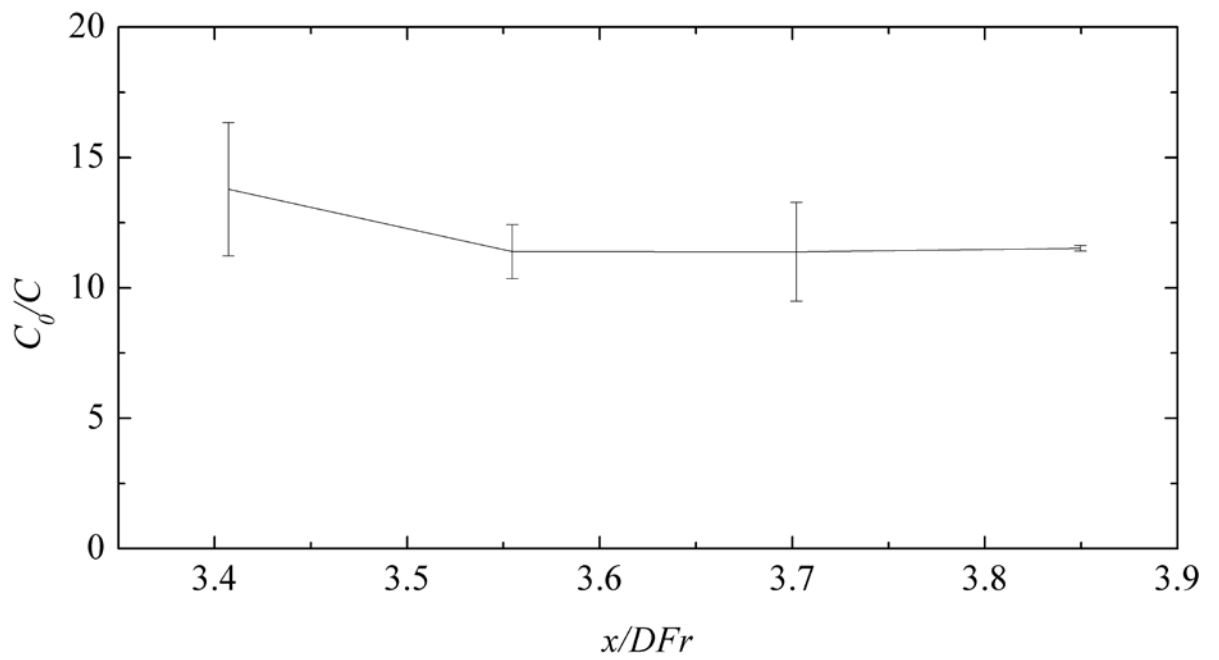


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Figure 3 (a) A structured mesh of the domain; (b) Detailed grids near the nozzle at the center plane

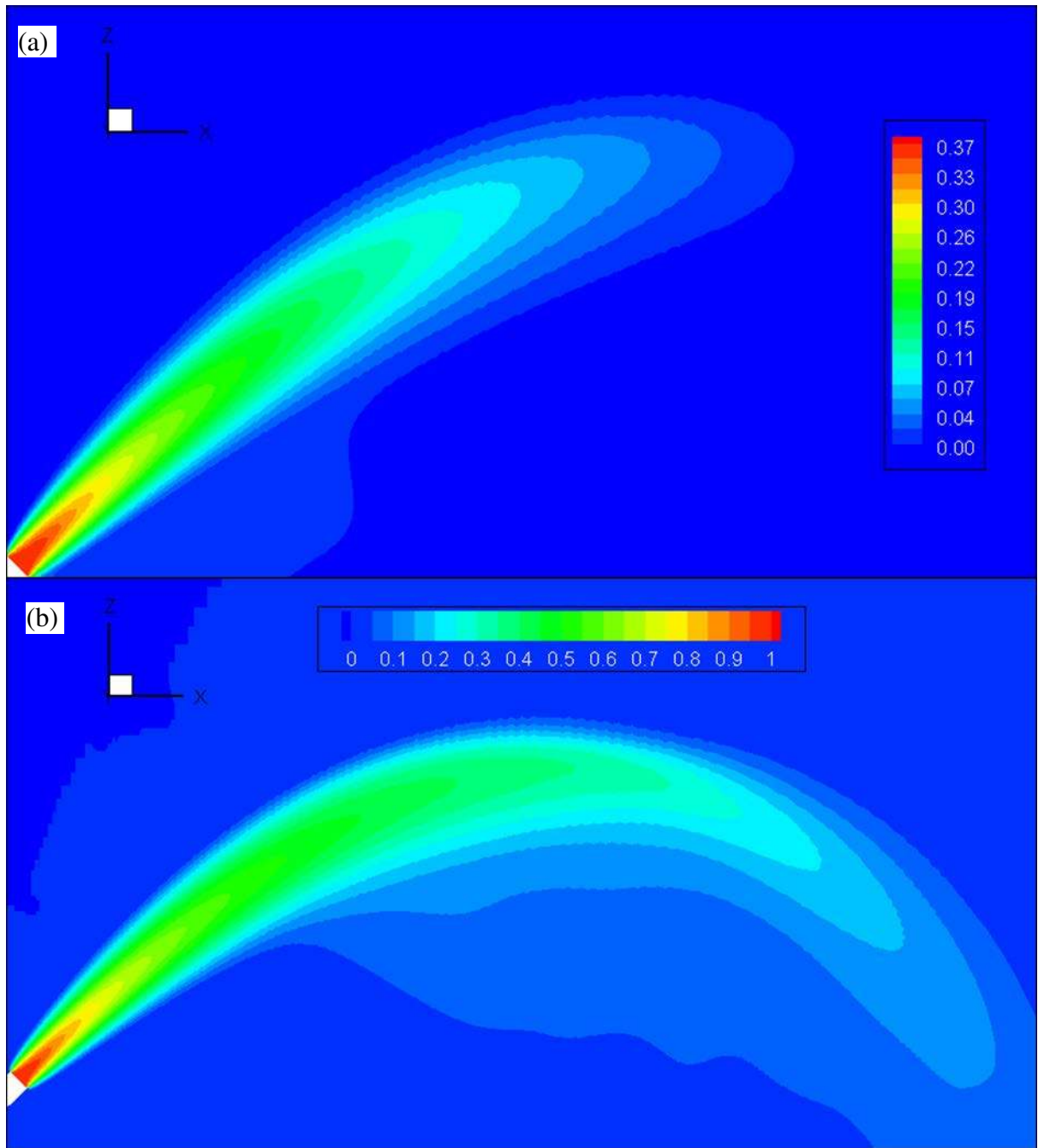


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Figure 4 Dilution at the nozzle height level near the return point

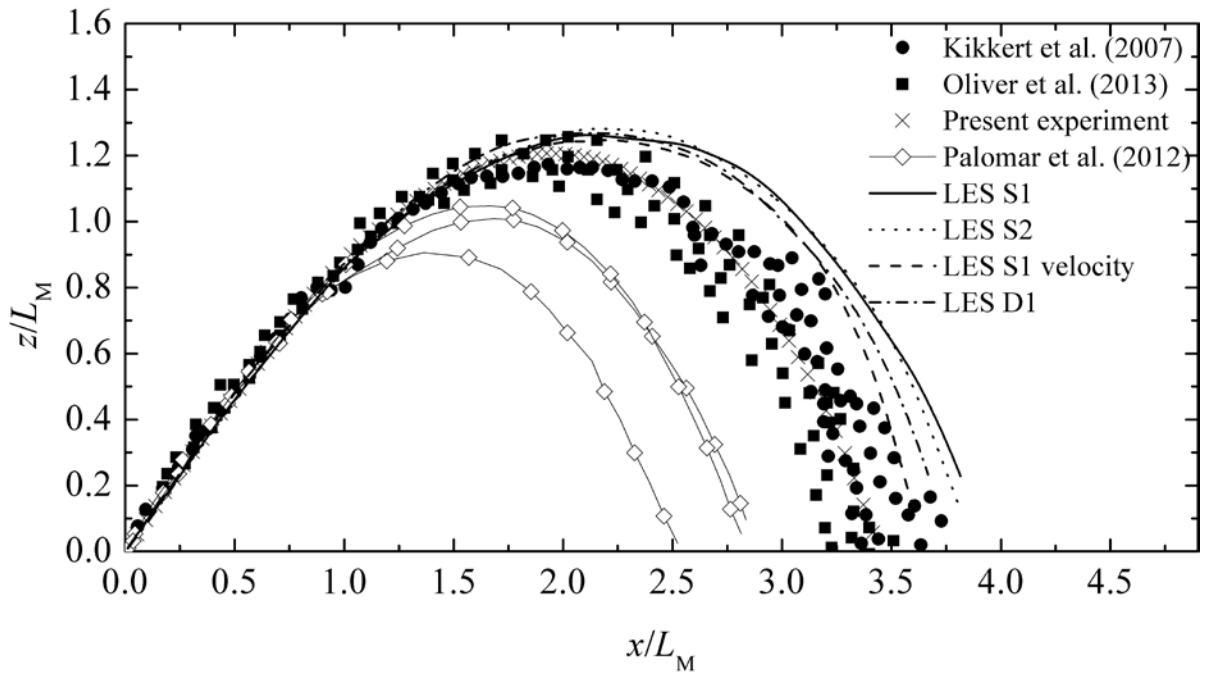




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2 Figure 5 Non-dimensional mean (a) velocity ( $m/s$ ) and (b) concentration contours  
 3 at the center plane for Case S1

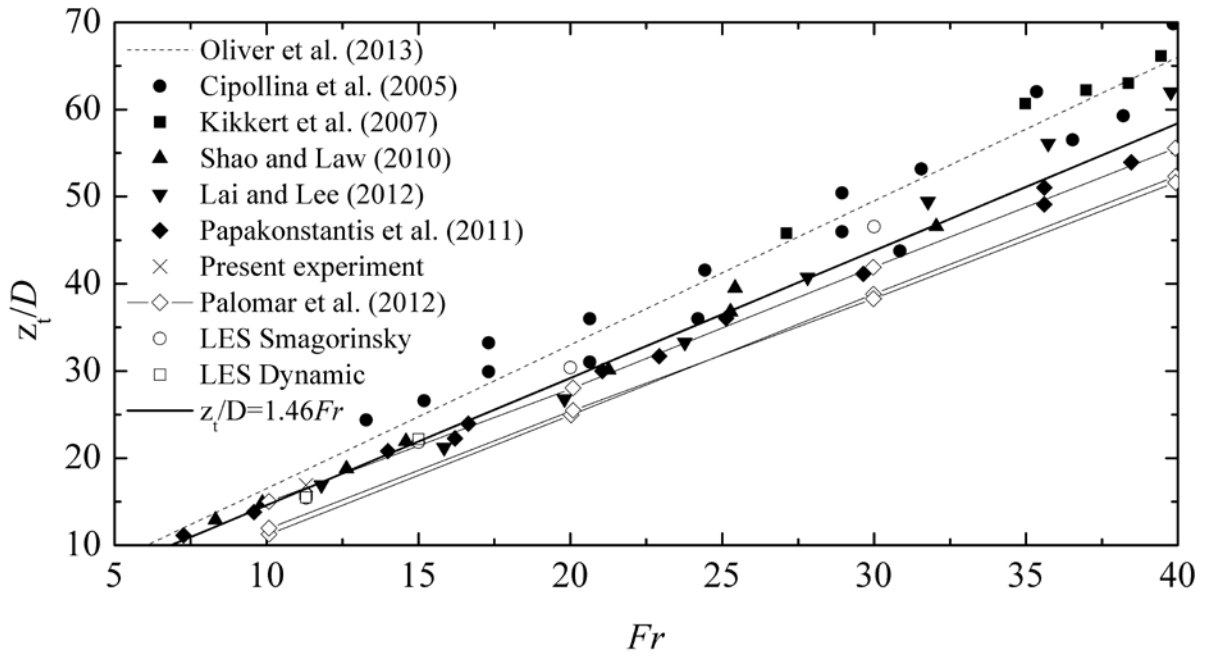
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Figure 6 Comparison of normalized centerline trajectories



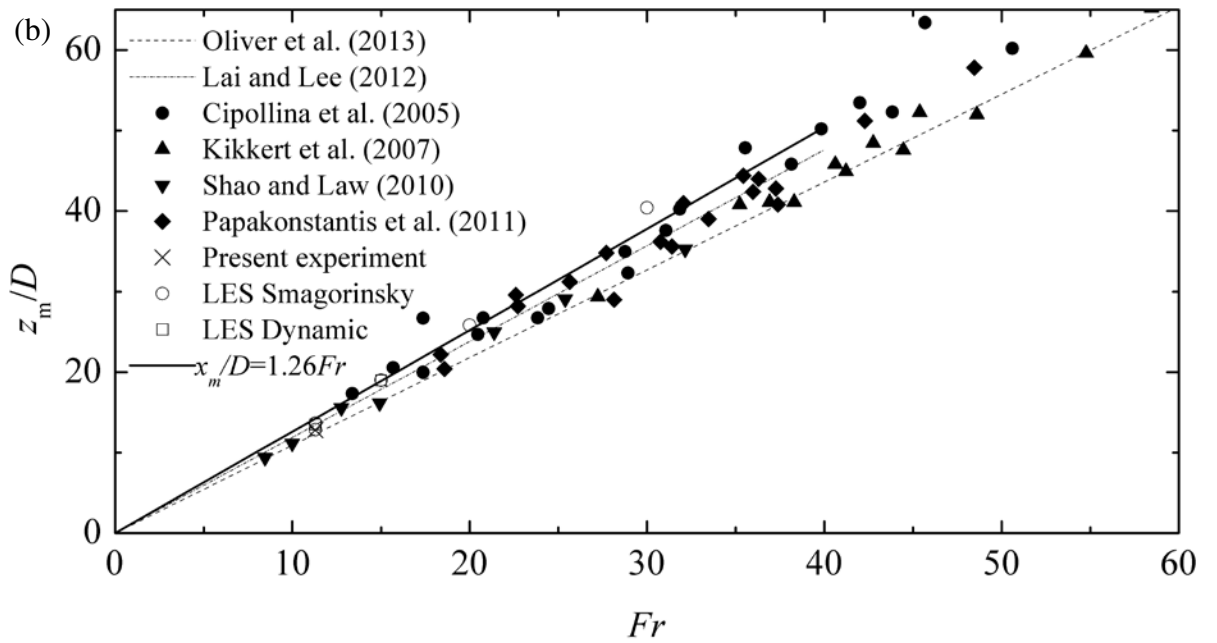
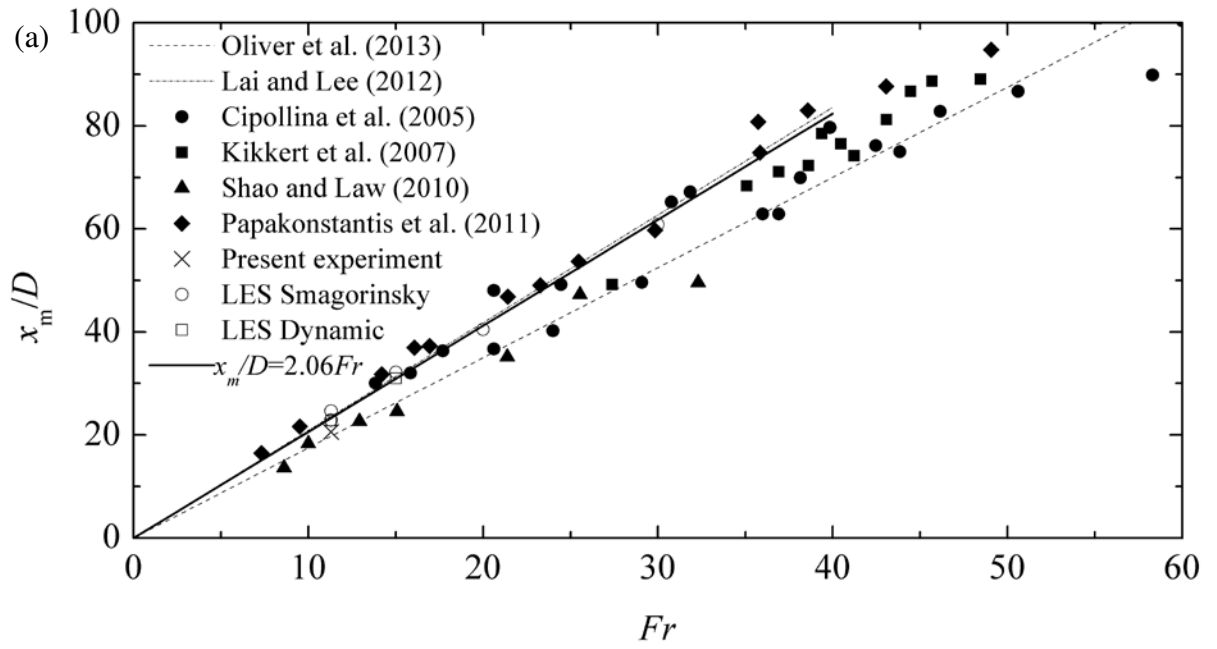
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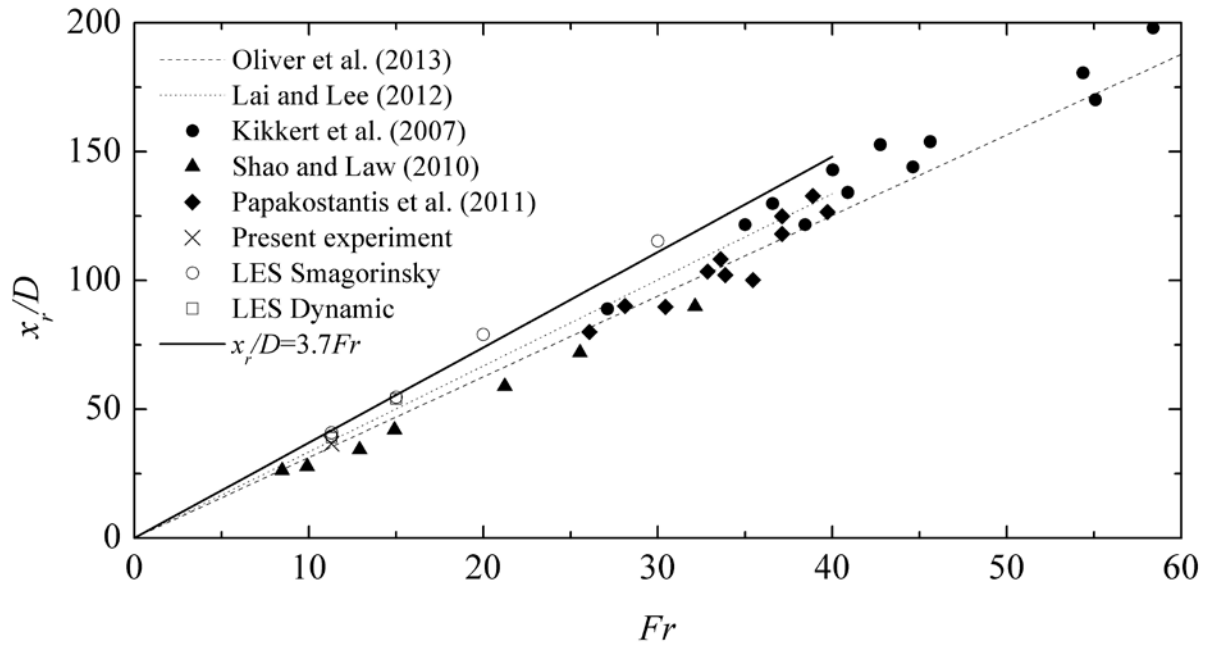
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Figure 7 Comparison of normalized terminal rise height



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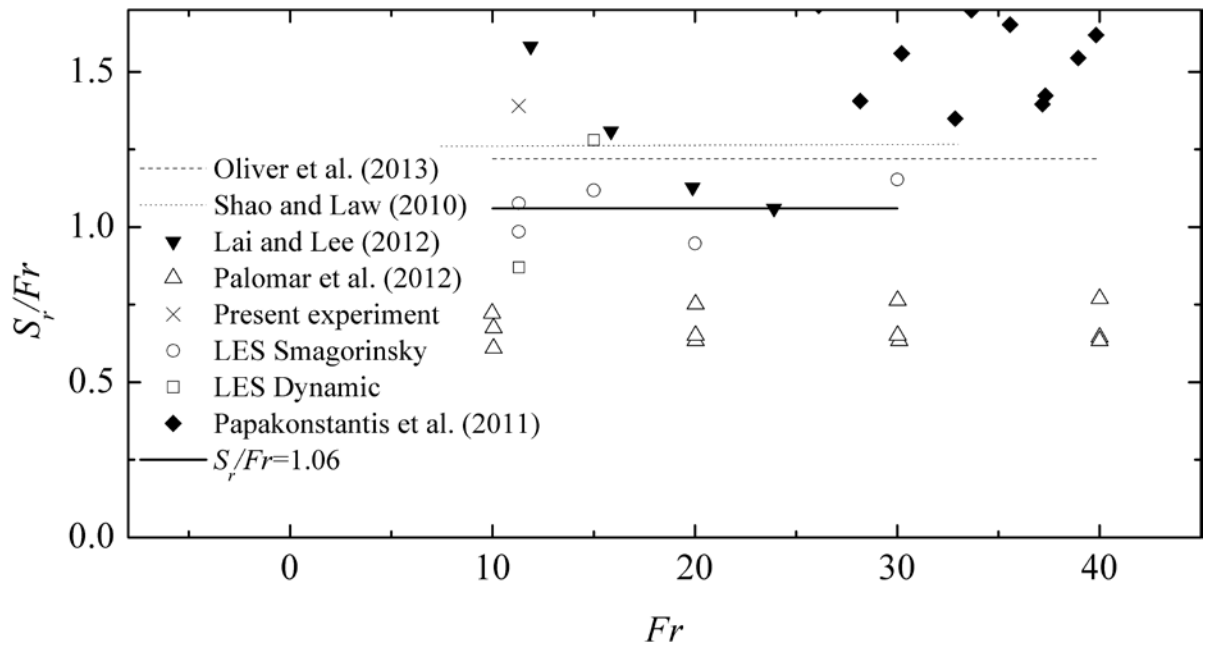
2 Figure 8 Comparison of normalized centerline peak: (a) horizontal and (b) vertical  
3 locations



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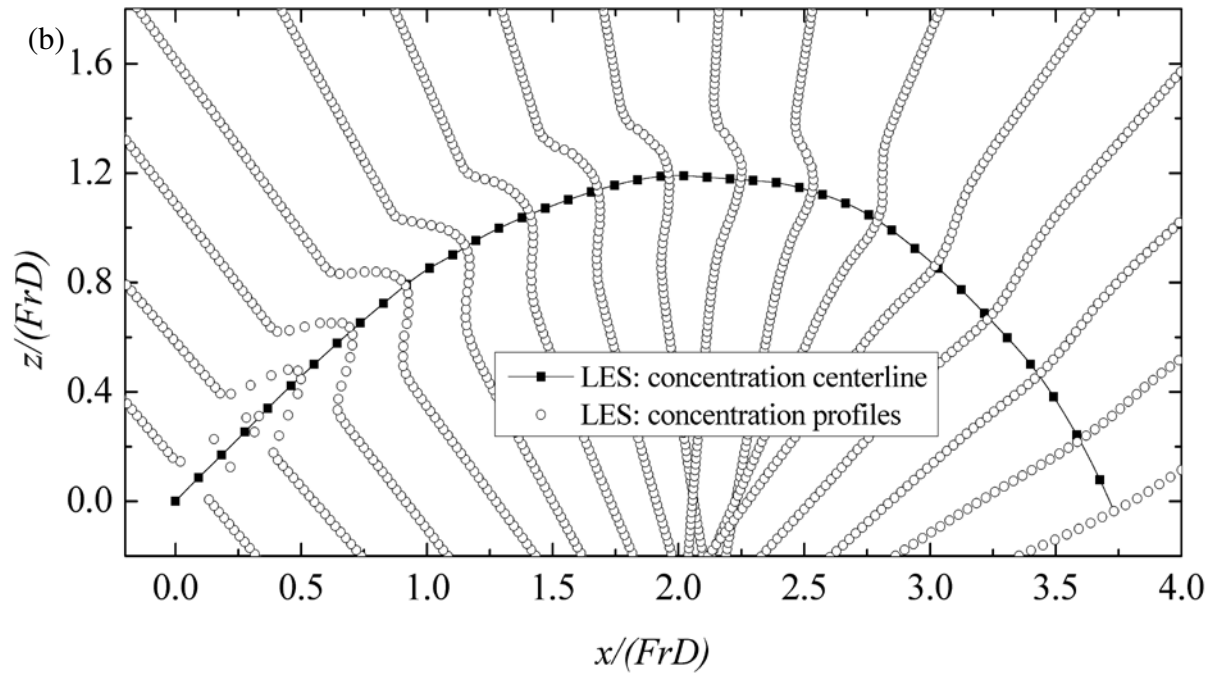
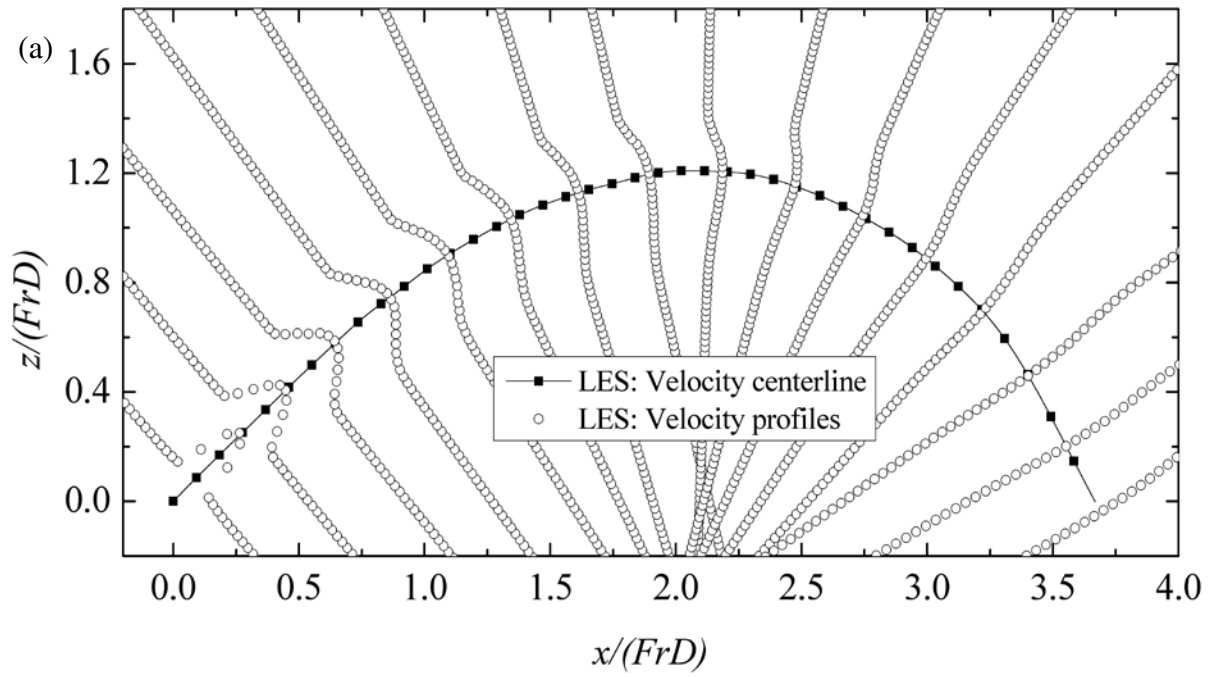
Figure 9 Comparison of normalized return point location



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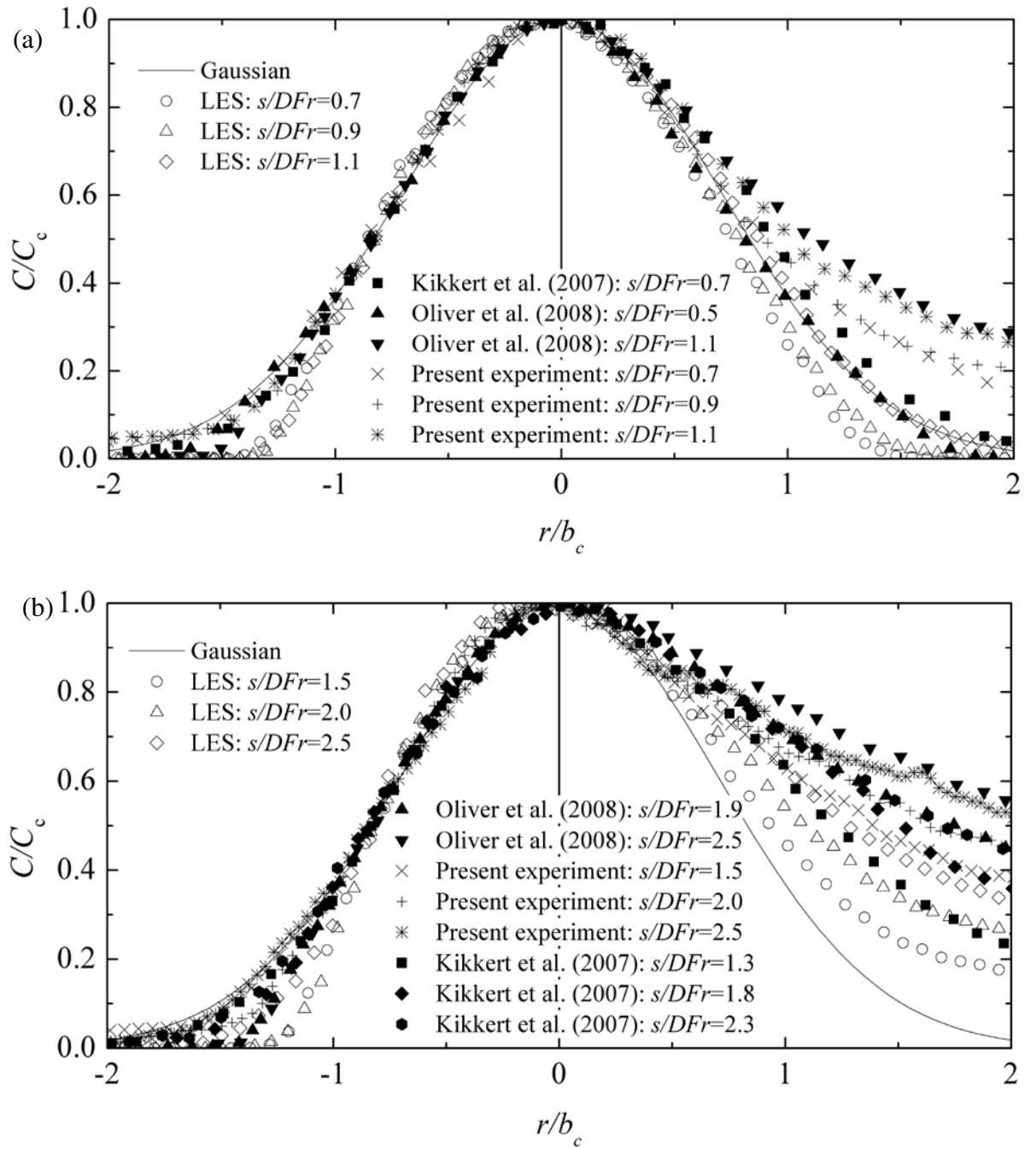
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Figure 10 Comparison of normalized dilution at the return point



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2 Figure 11 Cross-sectional profiles of (a) velocity and (b) concentration fields  
3 (Case S1)

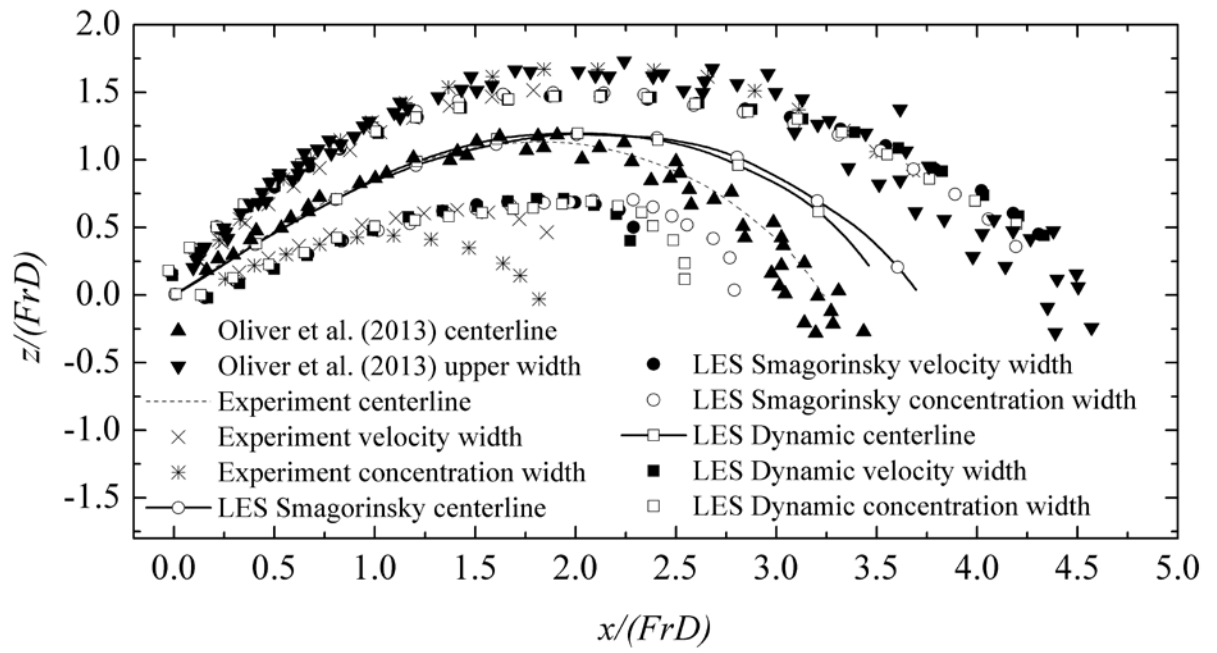


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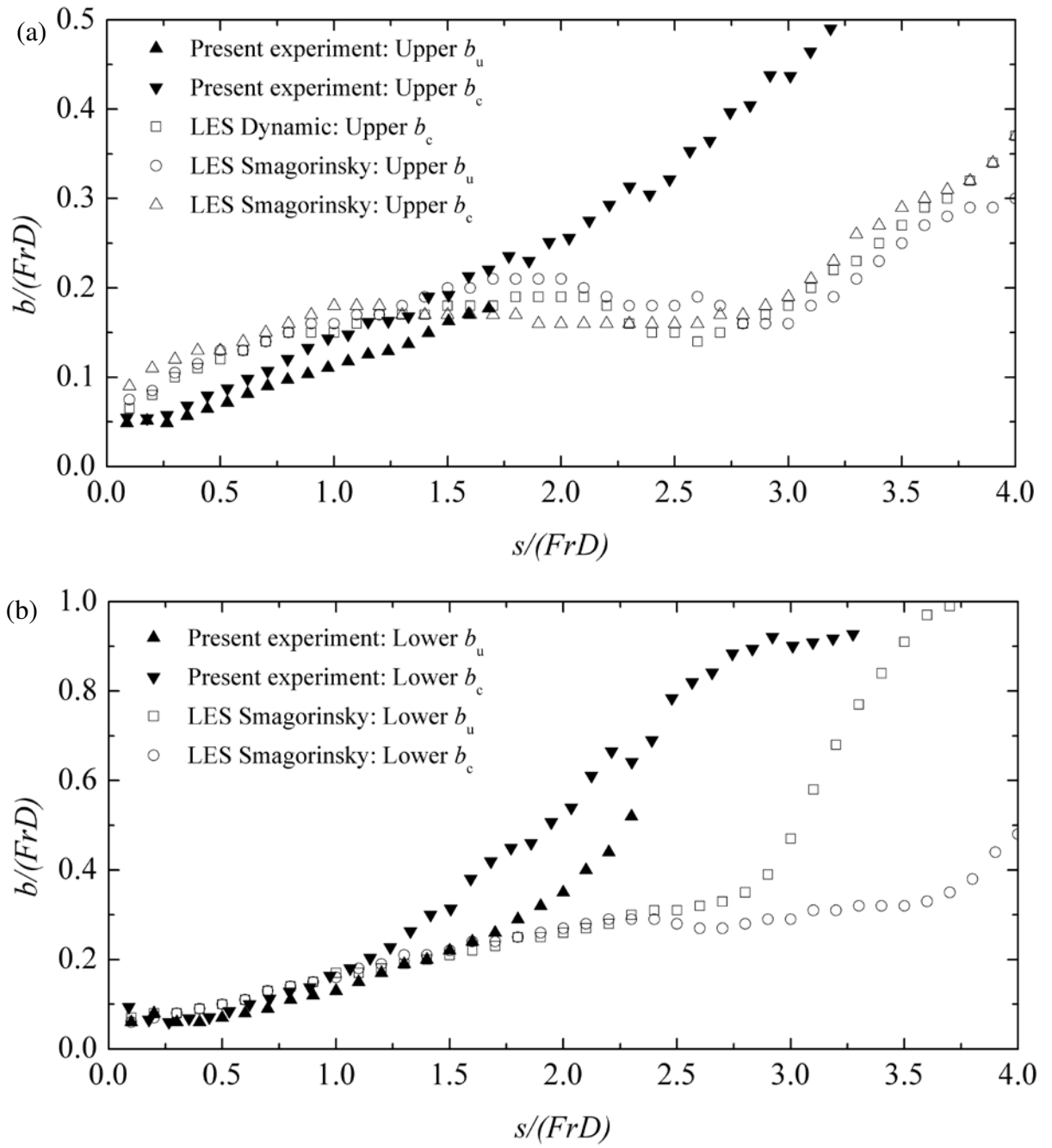
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Figure 12 Non-dimensional cross-sectional distributions of normalized concentration at (a)  $s/DFr = 0.5 \sim 1.2$  and (b)  $s/DFr = 1.2 \sim 2.5$



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2 Figure 13 Comparison of the jet velocity and concentration spread widths



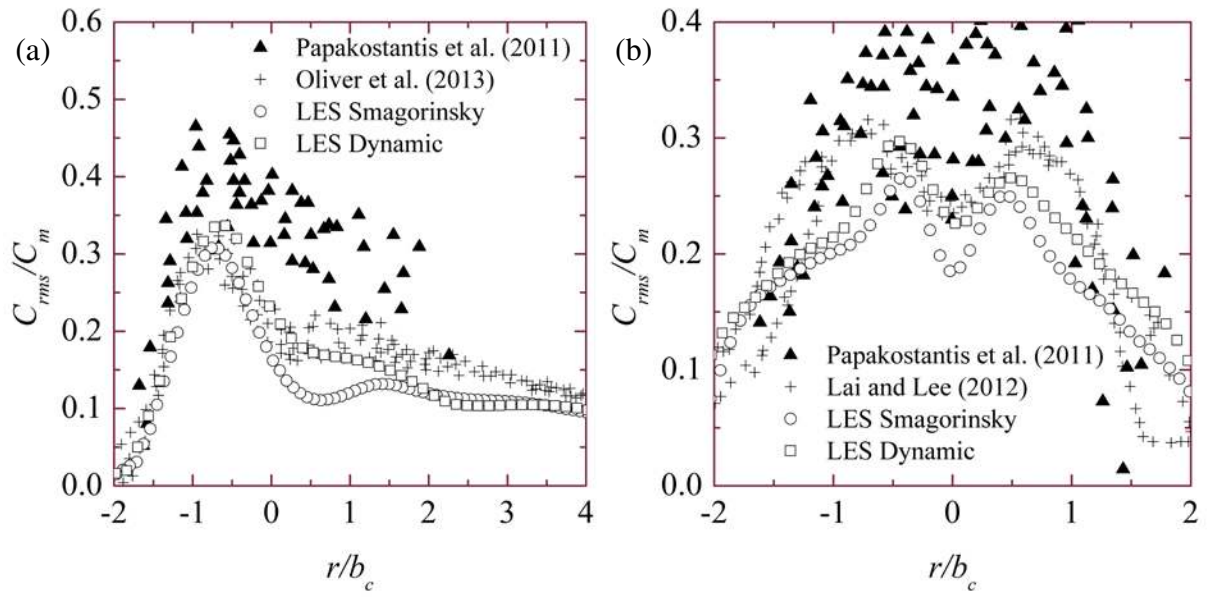
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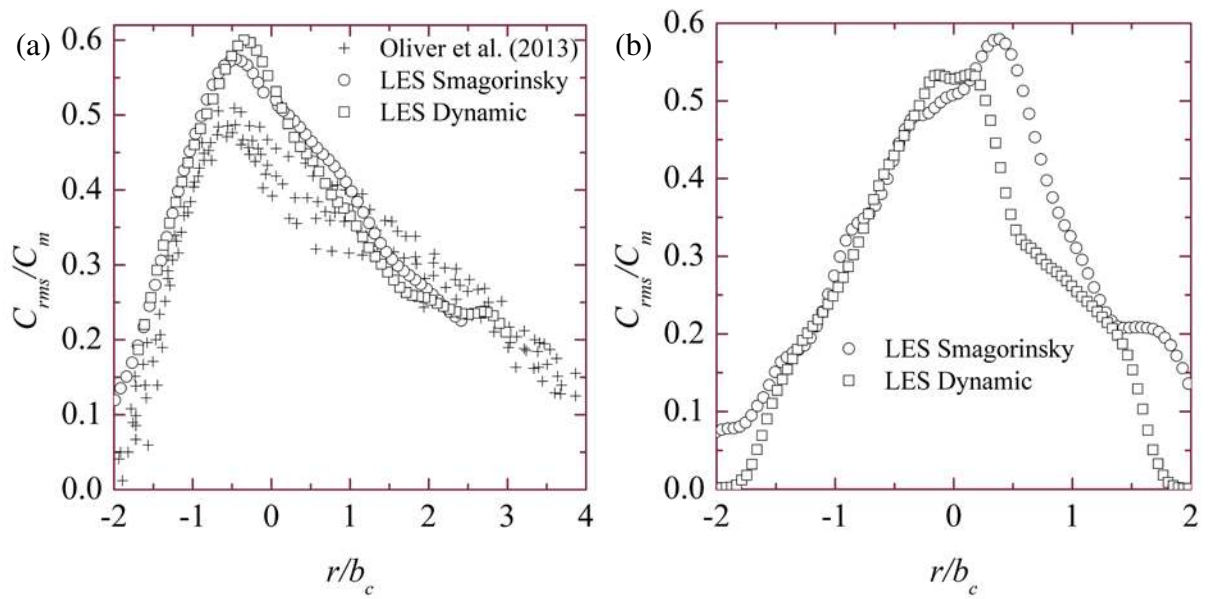
Figure 14 Variation of (a) upper and (b) lower jet spread widths along the trajectory





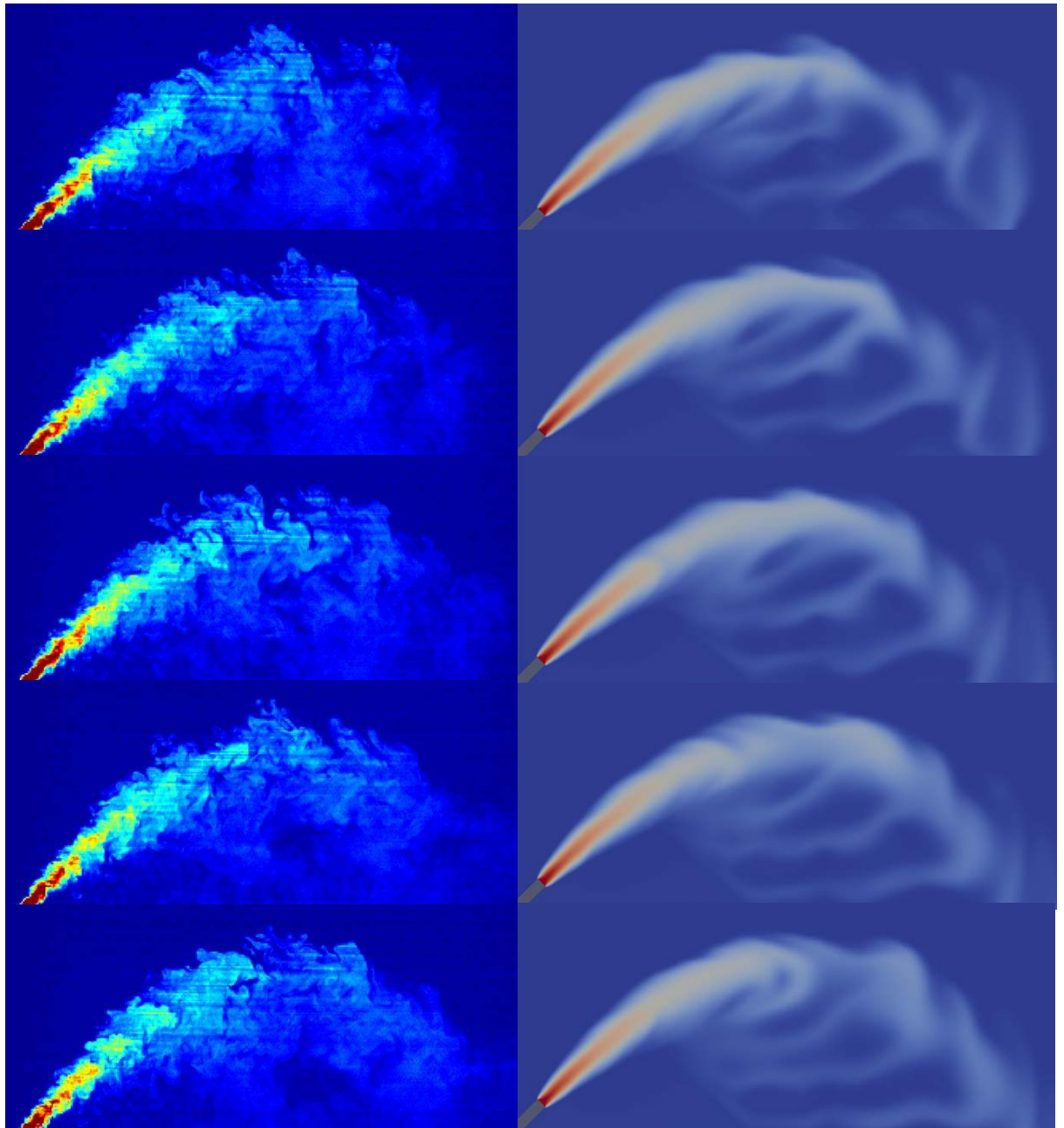
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2 Figure 15 Concentration turbulence intensity at the centerline peak in the (a)  
 3 vertical and (b) lateral directions



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5 Figure 16 Concentration turbulence intensity at the return point in the (a)  
 6 azimuthal and (b) lateral directions



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Figure 17 Eddy structures at the central plane: (Left) experimental images;  
(Right) LES predictions (Case S1)

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Table 1 Parameters and mesh sizes

Cases	Diameters (mm)	Velocity (m/s)	Brine density (kg/m <sup>3</sup> )	Ambient density (kg/m <sup>3</sup> )	<i>Fr</i>	Number of grid cells (Million)	SGS model
S1	6.0	0.513	1032	997	11.3	2.5	Smagorinsky
S2	6.0	0.679	1032	997	15.0	3.3	Smagorinsky
S3	6.0	0.909	1032	997	20.0	5.6	Smagorinsky
S4	6.0	0.909	1013	997	30.0	10.1	Smagorinsky
S5	8.0	0.547	1027	997	11.3	3.1	Smagorinsky
D1	6.0	0.513	1032	997	11.3	2.5	Dynamic
D2	6.0	0.679	1032	997	15.0	3.3	Dynamic
Present experiment	5.8	0.515	1034	997	11.3	--	--

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Table 2 Comparison of coefficients

Quantities	$\frac{x_m}{DFr}$	$\frac{z_m}{DFr}$	$\frac{z_t}{DFr}$	$\frac{x_r}{DFr}$	$\frac{S_m}{Fr}$	$\frac{S_r}{Fr}$	Bottom boundary	
LES (Smagorinsky)	2.06 $\pm 0.12$	1.26 $\pm 0.13$	1.46 $\pm 0.09$	3.71 $\pm 0.19$	0.26 $\pm 0.03$	1.06 $\pm 0.09$	No	
LES (Dynamic)	2.03	1.22	1.43	3.57	0.27	1.02	No	
Present experiment	1.82	1.13	1.68	3.24	0.41	1.49	No	
Kikkert et al. (2007)	1.84	1.06	1.60	3.26	-	-	No	
Oliver et al. (2013)	1.75	1.09	1.65	3.13	0.39	1.22	No	
Palomar et al. (2012)	CORJET	1.52	0.99	1.41	2.65	-	0.65	No
	UM3	1.32	0.85	1.24	2.32	-	0.63	No
	JETLAG	1.52	0.95	1.27	2.68	-	0.76	No
Cipollina et al. (2005)	1.80	1.17	1.61	2.82	-	-	Yes	
Shao and Law (2010)	1.69	1.14	1.47	2.83	0.46	1.26	Yes	
Papakonstantis et al. (2011a & b)	2.03	1.17	1.58	3.78	0.52	1.55	Yes	
Lai and Lee (2012)	2.09	1.19	1.58	3.34	0.45	1.09	Yes	

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