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1 Lattice-Boltzmann modeling of buoyancy-driven turbulent flows

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The pressure-based hybrid lattice-Boltzmann method presented by Farag & al in Phys. Fluids, vol. 32, p. 066106 (2020) is assessed for the simulation of buoyancy driven flows. The model is first validated on Rayleigh-Benard and Rayleigh-Taylor two-dimensional cases. A large-eddy simulation of a turbulent forced plume is then carried out, and results are validated against experiments. A good overall agreement is obtained, both for mean and fluctuations quantities, as well as global entrainment. The self-similarity characteristic of the plume in the far-field is also recovered.

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7 INTRODUCTION

8 Lattice Boltzmann Methods (LBM) are a powerful tool for the simulation of fluid
9 dynamics¹. Due to its attractive computational cost², its capacities for massively paral-
10 lel computing and the ease to deal with complex geometries using multi-level Cartesian
11 grids, these methods have attracted growing interest both in the academic and industrial
12 spheres in the past decade³⁻⁵.

13 LBM being initially designed to tackle isothermal flows, extension to thermal flows is to-
14 day an active topic of investigation in the community. In achieving that goal, the numerical
15 stability of the collision operator, at the heart of the method, used to be a major issue. The
16 single relaxation time Bhatnagar-Gross-Krook model⁶, probably the most popular model,
17 lacks stability for shear flows, but more recent models such as multiple relaxation collision⁷
18 or regularized kernels^{8,9} significantly improved stability. Another issue is the resolution of
19 energy or temperature equation, which cannot be straightforwardly achieved on low-order
20 lattices⁵. Two main options are available in the literature. The first is the double distribution
21 function (DDF) option that consists in coupling the LBM solver with a second distribution
22 function, whose main order corresponds to either temperature, energy, or enthalpy (see,
23 e.g.^{10,11}, for recent studies). A second option is to couple directly LBM with a scalar (tem-
24 perature, energy, enthalpy), solved in a coupled finite difference solver. This second option
25 was found attractive, as it allows, for a reasonable cost², to include an arbitrary number
26 of additional scalar equations. Following recent successful applications to compressible¹²⁻¹⁷,
27 atmospheric¹⁸⁻²² or reactive flows²³⁻²⁵, the second option, often referred to as hybrid LBM
28 is retained for this study. This work aims at investigating their applicability to buoyancy
29 driven flows, such as those encountered in fire-related problems²⁶.

30 The far field of turbulent, axisymmetric, free-plume in a quiescent, unstratified environ-
31 ment, where buoyancy-driven plume exhibits self-similar behavior, play a significant role in
32 various fluid flows of environmental and technological importance, including thermal plumes
33 that arise due to the convective heating on Earth's surface²⁷⁻²⁹, fire protection engineering
34 with problems associated with fire detection, smoke filling rates of indoor spaces, fire vent-
35 ing, fire heating of structural elements of buildings³⁰, wildland fires^{31,32}, dispersal of volcanic
36 eruptions³³⁻³⁵, sea ice plumes^{36,37}, smoke stacks³⁸, and cooling tower plume dispersion³⁹.
37 Forced plumes or buoyant jets represent a canonical configuration to study such plumes.

38 They consist by releasing the plumes from a source with some initial momentum. The flow
39 can be decomposed into three regions: (i) a region featuring a jet-like behavior near the
40 source, (ii) a transitional region and (iii) further downstream, the far-field fully-developed
41 buoyancy-driven plume⁴⁰.

42 The first far-field plume theories^{41–43} assumed a turbulent flow, a point source of buoyancy,
43 the Boussinesq approximation and a dynamic similarity of the mean and turbulent motion
44 at all elevations. Morton et al.⁴³ developed an integral formulation by assuming both “top-
45 hat” radial profiles for both velocity and temperature (density) and a point source, and
46 by introducing an entrainment coefficient, α , defined as the ratio of radial velocity at the
47 edge of the plume to the vertical velocity within the plume. Their model predicts correctly
48 the scaling laws for the plume radius, that increases linearly with height, z , as well as
49 for both velocity and temperature rise above the ambient that decay as $z^{-1/3}$ and $z^{-5/3}$,
50 respectively. The weak plume formulation of Morton et al.⁴³ was extended to “strong plumes”
51 by removing both the Boussinesq approximation and the point source assumption through
52 the introduction of a virtual origin and, by considering more realistic Gaussian profiles for
53 both velocity and temperature³⁰. This in conjunction with experiments in fire plumes above
54 the flames⁴⁴ provided expressions for plume radius and centreline velocity and temperature
55 consistent with experimental data^{45–47}. Another important feature of buoyant plumes is
56 that the radial profiles of dimensionless mean velocity and temperature and dimensionless
57 rms turbulent fluctuations of velocity and temperature exhibit a self-similar behaviour with
58 $\eta = r/z$ as a self-similar variable, where r is the radial coordinate^{45–49}. Progress was also
59 made in the understanding of the role of buoyancy on the entrainment process and the flow
60 behavior. In particular, Saeed et al. found that buoyancy contributes to enhance the mean
61 kinetic energy budget but also the momentum flux⁵⁰.

62 The CFD modeling of forced plumes was also a very active research area. A significant
63 amount of Reynolds-Averaged Navier-Stokes simulations were reported with different for-
64 mulations of the $k-\epsilon$ model^{51–54}. On the other hand, Zhou et al.⁵⁵ and Yan⁵⁶ showed the
65 capability of Large Eddy Simulation (LES) to predict well the plume’s puffing, self-preserving
66 and spreading. LES of forced jet were also performed⁵⁷ to evaluate the energy-consistent
67 approach for modeling entrainment rate coefficient, α , developed by Kaminski et al.⁵⁸ and
68 van Reeuwijk and Craske⁵⁹. Direct numerical simulation (DNS) and LES of thermal plumes
69 were also reported^{60–63}. These studies focused mainly on the generation and growth of

70 buoyancy-induced instabilities in the near field that governs the transition from laminar to
71 turbulence. In particular, it was shown that these instabilities have to be fully resolved to
72 capture the dynamics of such purely buoyant thermal plumes⁶⁰. In addition, the DNS was
73 found in good agreement with experimental data in the far field⁶¹.

74 This literature survey reveals that all the numerical investigations were performed by
75 using a low Mach-formulation of the Navier-Stokes equation. To the authors' best knowledge,
76 no attempt to consider lattice-Boltzmann method was reported.

77 The goal in the current work is to assess the ability of the pressure-based Lattice-
78 Boltzmann method proposed by Farag et al.¹⁶ to correctly predict the behavior of a forced
79 plume in the self-similarity region away from the source. This manuscript is organized as
80 follows. The first Section recalls the target macroscopic equations, as well as the Lattice-
81 Boltzmann algorithm proposed. The second Section presents a number of 2D canonical
82 flow validations, including Rayleigh-Benard and Rayleigh-Taylor instabilities. The third
83 Section presents a large eddy simulation of the plume experimentally described by Shabbir
84 and George⁴⁷, along with comparisons with the large eddy simulation presented by Zhou et
85 al.⁵⁵ and the theoretical model of Morton^{28,43}. All the simulations were performed using the
86 compressible ProLB code⁶⁴.

87 I. LATTICE-BOLTZMANN MODEL FOR COMPRESSIBLE FLOWS

88 A. Macroscopic governing equations

89 The flow mass, momentum and energy conservation equations are introduced as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j + \delta_{ij} p}{\partial x_j} = \frac{\partial \Pi_{ij}}{\partial x_j} + \rho g_i, \quad (i = 1, 2, 3) \quad (2)$$

$$\rho \frac{\partial h}{\partial t} + \rho u_j \frac{\partial h}{\partial x_j} = \frac{Dp}{Dt} - \frac{\partial q_j}{\partial x_j} + \Pi_{ij} \frac{\partial u_i}{\partial x_j}, \quad (3)$$

90 where ρ is the mass volume, u_i is the velocity vector, p is the pressure, g_i is the gravitational
91 acceleration, h is the mass enthalpy and δ_{ij} as the Kronecker delta symbol. Throughout
92 this manuscript, we neglect the pressure work $\frac{Dp}{Dt} = \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} \approx 0$ in the energy equation,
93 a reasonable approximation for buoyancy driven flows. The stress tensor Π_{ij} in Eqs. (2-3)

94 reads

$$\Pi_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \delta_{ij} \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right), \quad (4)$$

95 with μ the dynamic viscosity. Finally, the heat flux q_i in the energy equation reads

$$q_i = -\lambda \frac{\partial T}{\partial x_i} \quad (5)$$

96 where T is the temperature, and λ the heat conductivity, obtained assuming constant Prandtl
97 number:

$$\text{Pr} = \frac{c_p \mu}{\lambda} = \frac{\nu}{\alpha}, \quad (6)$$

98 where ν is the kinematic viscosity defined as $\nu = \mu/\rho$ while α is the thermal diffusivity
99 defined as $\alpha = \lambda/\rho c_p$. The system of Eqs (1-3) is fully closed by the choice of an equation
100 of state

$$p = \rho r T, \quad h = c_p T, \quad (7)$$

101 with c_p the mass heat capacity at constant pressure, and $r = 287 \text{J kg}^{-1} \text{K}^{-1}$ is the gas
102 constant for air per unit mass. Note that we assume c_p to be constant, since the temperature
103 in the test cases presented does not exceed 600K.

104 B. Turbulence modeling

105 For the large eddy simulation presented in Sec. III, a Vreman eddy-viscosity subgrid scale
106 model is used⁶⁵. The filtered expressions for Eqs. (1-3) are widely reported in the literature
107 (see, e.g.⁶⁶) and not recalled here. Applying the subgrid-scale model numerically comes
108 down to modifying the viscosity μ through the addition of a turbulent viscosity μ_t obtained
109 as:

$$\mu_t = \rho C \sqrt{\frac{B_\beta}{\alpha_{ij} \alpha_{ij}}}, \quad (8)$$

with

$$\alpha_{ij} = \frac{\partial u_j}{\partial x_i}, \quad (9)$$

$$\beta_{ij} = \Delta_m^2 \alpha_{mi} \alpha_{mj}, \quad (10)$$

$$B_\beta = \beta_{11} \beta_{22} - \beta_{12}^2 + \beta_{11} \beta_{33} - \beta_{13}^2 + \beta_{22} \beta_{33} - \beta_{23}^2, \quad (11)$$

110 The constant C is related to the Smagorinsky constant C_s as $C = 2.5 C_s^2$. Δ_m is the
111 local mesh size. The model is simple to implement and compute as it only requires the

112 local filter width (i.e. mesh size) and the first order derivatives of the velocity field. In our
 113 simulation $C_s = 0.1$, following Vreman's recommendation⁶⁵, which was also adopted in the
 114 forced plume large eddy simulation by Zhou et al.⁵⁵. The heat flux takes into account the
 115 subgrid contribution via a turbulent Prandtl number Pr_t .

116 C. Numerical method: Lattice Boltzmann solver

117 For a complete description of the numerical method, the reader is referred to Farag et
 118 al.^{16,17}. Lattice-Boltzmann methods are derived from a space, time and velocity discretiza-
 119 tion of the Boltzmann equation⁵. In the present model, the probability density function f_i
 120 is solved at each point x via the Boltzmann equation discretized as:

$$f_i(x + c_i \delta t, t + \delta t) = f_i^{\text{eq}}(x, t) + \left(1 - \frac{\delta t}{\tau}\right) f_i^{\text{neq}}(x, t) + \frac{\delta t}{2} F_i^E(x, t) \quad (12)$$

121 where δt is the time-step, and c_i is the i^{th} discrete velocity of the D3Q19 lattice⁶⁷, and F_i^E
 122 is a volume force including gravity and correcting terms, as defined in Appendix A. The
 123 equilibrium and off-equilibrium populations ($f_i^{\text{eq}}, f_i^{\text{neq}}$) are to be defined in Eqs (14, 16).

124 In Eq. (12), the relaxation time τ is related to the dynamic viscosity as:

$$\tau = \frac{\mu}{\rho c_s^2} + \frac{\delta t}{2}, \quad (13)$$

125 where $c_s = \delta x / (\sqrt{3} \delta t)$ is the characteristic velocity of the D3Q19 lattice⁶⁷.

126 The equilibrium function is obtained as:

$$f_i^{\text{eq}} = \omega_i \left(\rho \theta + \frac{\mathcal{H}_{i,\alpha}^{(1)}}{c_s^2} \rho u_\alpha + \frac{\mathcal{H}_{i,\alpha\beta}^{(2)}}{2c_s^4} \rho u_\alpha u_\beta + a^{(3)} + a^{(4)} \right), \quad (14)$$

127 where ω_i is the D3Q19 weight of discrete velocity c_i , \mathcal{H}_i are the discrete Hermite polynomials,
 128 defined in Appendix A, and $a^{(3)}$ and $a^{(4)}$ are third and fourth order terms also provided in
 129 Appendix A. The reduced temperature θ reads

$$\theta = \frac{rT}{c_s^2}. \quad (15)$$

130 The off-equilibrium counterpart f_i^{neq} is obtained as:

$$f_i^{\text{neq}} = \omega_i \left[\frac{\mathcal{H}_{i,\alpha\beta}^{(2)}}{2c_s^4} a_{\alpha\beta}^{(2),\text{neq}} + \frac{\mathcal{H}_{i,\gamma}^{(3r)}}{6c_s^6} a_\gamma^{(3r),\text{neq}} \right], \quad (16)$$

131 with

$$a_{\alpha\beta}^{(2),\text{neq}} \equiv a_{\alpha\beta}^{*(2),\text{neq}} - \frac{\delta_{\alpha\beta}}{3} a_{\gamma\gamma}^{*(2),\text{neq}}, \quad (17)$$

$$a_{\alpha\beta}^{*(2),\text{neq}} = \sum_i \left[\left(f_i - f_i^{\text{eq}} + \frac{\delta t}{2} F_i^E \right) \mathcal{H}_{i,\alpha\beta}^{(2)} \right]. \quad (18)$$

132 and the third-order contribution defined in Appendix A.

133 Finally, the macroscopic variables are reconstructed from f_i as:

$$\rho(t + \delta t, x) = \sum_i f_i(t + \delta t, x) - (\rho\theta)(t, x) + \rho(t, x) \quad (19)$$

$$\rho u_i(t + \delta t, x) = \sum_i c_i \left(f_i(t + \delta t, x) + \frac{\delta t}{2} F_i^g \right). \quad (20)$$

134 where F_i^g is the gravity force term defined in Appendix A. The enthalpy equation (3) is
 135 solved at the same time using a finite difference discretization under non-conservative form,
 136 exactly as presented by Tayyab *et al.*^{23,24}. Second-order consistency to the macroscopic
 137 equations (1-3) can be shown via Chapman-Enskog⁵, or Taylor^{68,69} expansions.

138 II. CANONICAL 2D VALIDATIONS

139 This Section provides canonical validations of the numerical method presented above.
 140 It focuses on two gravity-driven configurations: the Rayleigh-Benard and Rayleigh-Taylor
 141 instabilities, since the properties of the flow solver are already validated in a large number
 142 of compressible flow configurations in the absence of gravity^{2,16,17,19,24,25,70}.

143 A. Rayleigh-Benard Instability

144 The Rayleigh-Benard instability is a configuration involving natural convection and heat
 145 transfer⁷¹.

146 Figure 1 depicts the configuration to be simulated. It consists of a square box of dimension
 147 $1 \text{ m} \times 1 \text{ m}$ initially filled with quiescent air, and surrounded by adiabatic walls on the left
 148 and right, and isothermal top and bottom walls, resp. at $T_C = 299.5 \text{ K}$ and $T_H = 300.5 \text{ K}$.

149 The Rayleigh number, Ra, describes, on the one hand, the balance between buoyancy ver-
 150 sus viscous forces in the momentum equation and, on the other hand, the balance between

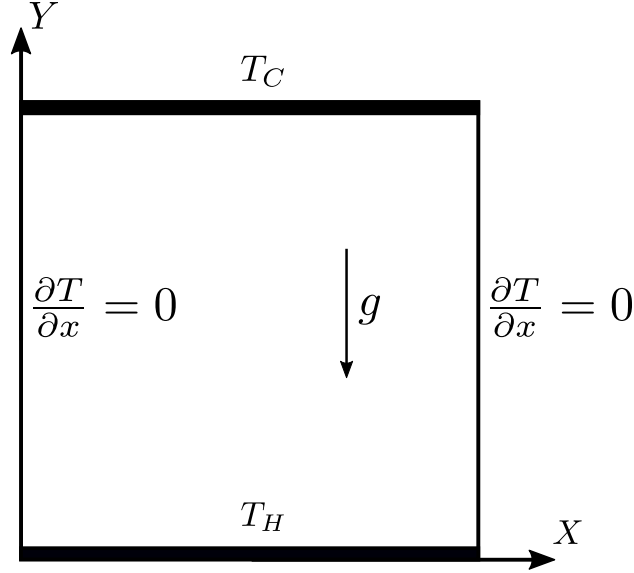


Figure 1: Schematic of Rayleigh Benard test case

151 conductive versus convective transfer in the energy equation. It is assumed that convec-
 152 tive heat transfer takes place with the velocity obtained by the balance in the momentum
 153 equation, and it is defined as:

$$\text{Ra} = \frac{g\beta(T_H - T_C)H^3}{\alpha\nu} = \text{Pr} \frac{g\beta(T_H - T_C)H^3}{\nu^2}, \quad (21)$$

154 where $g = 9.81\text{ms}^{-2}$ is the gravitational acceleration and $H = 1\text{ m}$ is the domain size. β
 155 is the thermal expansion coefficient that is equal to $1/T_{ref}$ for an ideal gas with isobaric
 156 expansion (i.e. at constant pressure). In the present study, T_{ref} is taken equal to T_H .
 157 Setting $\text{Pr} = 0.71$, the viscosity can be deduced from the target Rayleigh numbers (Eq. 21)
 158 of 10^4 , 10^5 and 10^6 , while the thermal conductivity, λ , in the energy equation is obtained
 159 from Eq. (6).

160 The domain is discretized with a uniform grid with 256×256 cells. The flow is then
 161 uniformly initialized as $u_0 = 0$, $T_0 = 300\text{K}$, $\rho_0 = 1.2\text{ kg m}^{-3}$, and $p = p_0 + \rho_0gy$. The
 162 simulation is then carried out until convergence using a time-step, $\delta_t = 6.5 \times 10^{-6}\text{ s}$.

163 Figure 2 presents temperature contours as well as streamline patterns, showing a good
 164 qualitative agreement with the literature (see⁷², e.g.): for $\text{Ra} = 10^4$, the flow is symmetric
 165 and dominated by the recirculation in the core region with small eddies near the corner.
 166 When increasing the Raleigh number, secondary eddies near the top left and bottom right
 168 corners appear and become larger.

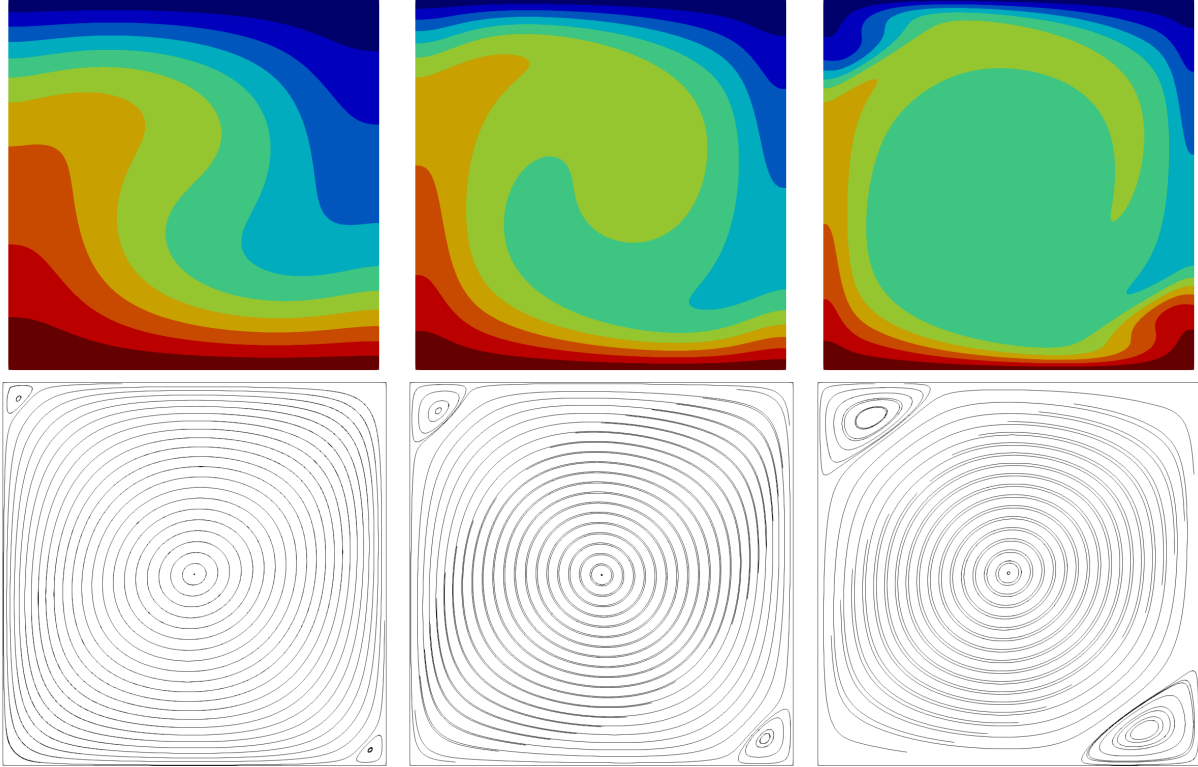


Figure 2: Rayleigh-Benard instability: Temperature contours (top) and streamlines (bottom), for three Rayleigh numbers (10^4 , 10^5 , 10^6), from left to right.

169 The quantitative agreement is shown in Fig. 3, presenting velocity profiles along the cen-
 170 terlines. The present numerical results are compared with the benchmark solution provided
 171 by Ouertatani et al.⁷². For further validation, the local Nusselt number Nu is calculated at
 172 the bottom wall as:

$$Nu = \left. \frac{\partial T}{\partial y} \right|_{y=0}. \quad (22)$$

173 It can be observed that both velocity and Nusselt number profiles are in excellent agree-
 174 ment with the reference solutions.

175 B. Rayleigh-Taylor instability

176 The Rayleigh-Taylor instability is another classical test case for buoyancy-driven flows
 177 due to its practical and fundamental importance. It was investigated extensively in the
 178 literature by different numerical methods^{73–82}. It consists of two layers of fluids of different
 179 densities (ρ_H, ρ_L) at rest under gravitational field, as illustrated in Fig. 4.

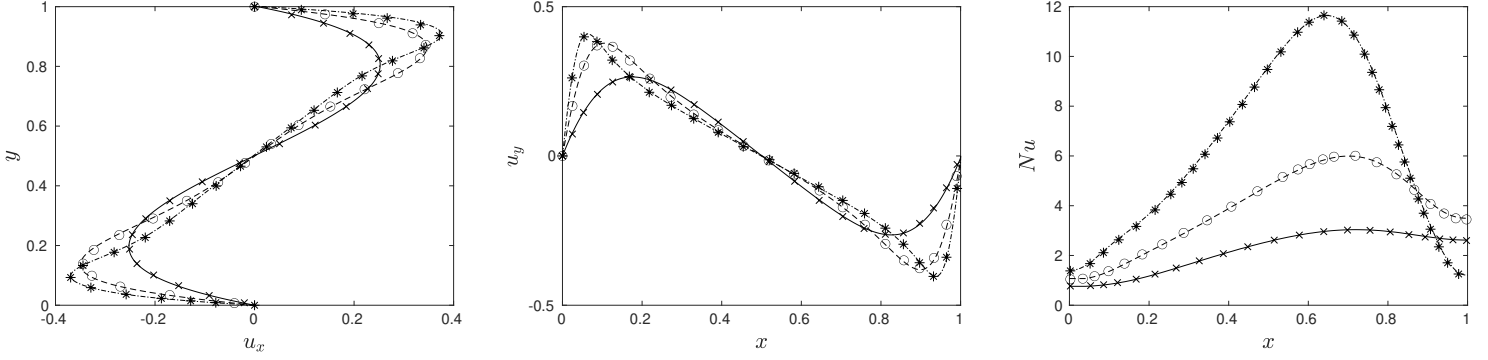


Figure 3: Rayleigh-Benard instability. u_x along the vertical centerline, u_y along the horizontal centerline, and Nusselt number along the bottom wall (from left to right), for $Ra=10^4$ (solid), $Ra=10^5$ (dashed) and $Ra=10^6$ (dot-dashed). Symbols indicate the reference data⁷²

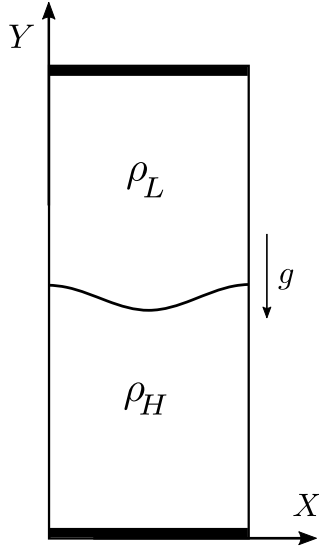


Figure 4: Schematic of Rayleigh Taylor instability.

180 The dynamics of this problem is governed by the Atwood (At) and Reynolds (Re) num-
 181 bers:

$$At = \frac{\rho_H - \rho_L}{\rho_H + \rho_L}, \quad Re = \frac{U^* L_x}{\nu}, \quad (23)$$

182 where L_x is the dimension of the domain in the horizontal direction and $U^* = \sqrt{gL_x}$ is a
 183 reference velocity.

184 The investigated configuration was previously studied in the literature⁷³⁻⁷⁵ with two target

185 Reynolds numbers of 256 and 2048, The domain size is $L_x \times 4L_x$, discretized with 256×1024
 186 (fine mesh) or 128×512 grid points (coarse mesh). The heavy (index H) and light (index
 187 L) fluids are initially separated by a perturbed interface given by the following equation:

$$y_i(x) = \frac{L_x}{10} \cos\left(\frac{2\pi x}{L_x}\right) + 2L_x \quad (24)$$

188 The fluids initial densities are set to $\rho_H = 3 \text{ kg m}^{-3}$ and $\rho_L = 1 \text{ kg m}^{-3}$, corresponding to
 189 $At=0.5$. The pressure was initialized to account for the gravity field as follows:

$$p = \begin{cases} p_0 + \rho_L g y, & 0 \leq y \leq y_i(x) \\ p_0 + \rho_L g y_i(x) + \rho_H g (y - y_i(x)), & y_i(x) < y \end{cases} \quad (25)$$

190 where p_0 is the pressure at $y = 0$. Finally, the domain size and gravity are set to $L_x = 0.25\text{m}$
 191 and $g = 20\text{m s}^{-2}$. The fluid viscosity is obtained from the target Reynolds numbers of 256
 192 and 2048.

193 Figure 5 represents the density contours obtained for the two Reynolds numbers of 256
 194 and 2048 using the finer mesh. The diagrams of the right of the figure represents the time
 195 evolution of the bubble and spike positions. Numerical predictions are compared to reference
 196 numerical simulation⁷³, showing an excellent agreement.

198 To investigate the robustness of the method, simulations were carried out on the coarser
 199 mesh. An excellent agreement is also obtained with a maximum error less than 2%.

200 III. LARGE EDDY SIMULATION OF A THERMAL PLUME

201 This Section presents a large eddy simulation of a buoyant plume, generated by a vertical
 202 jet of hot air into a quiescent atmosphere. The source conditions correspond to the experi-
 203 ments of Shabbir and George⁴⁷, summarized in Table I. The plume source diameter, D , the

$D(m)$	$T_a(K)$	$T_0(K)$	$U_0(m/s)$	$F_0(m^4/s^3)$	$M_0(m^4/s^3)$	$Re = \frac{U_0 D}{\nu}$	$Fr = \frac{U_0^2}{gD}$
0.0635	300	568	0.98	0.0127	0.003	1273	1.54

Table I: Source parameters of the plume

204

205

206 exit mean velocity, U_0 , the hot air temperature, T_0 , and the ambient air temperature, T_a , are
 207 6.35 cm, 0.98 m/s, 568 K and 300 K, respectively. The corresponding Reynolds number, Re ,

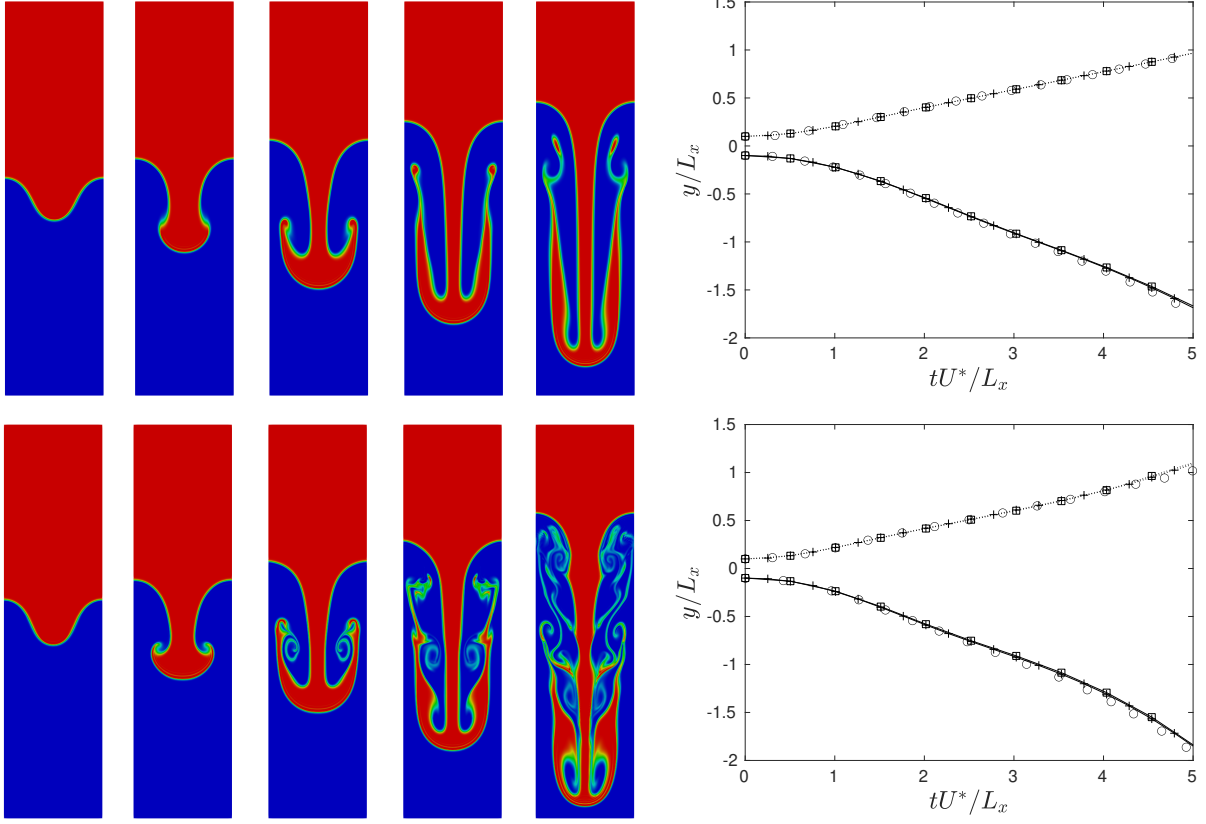


Figure 5: Rayleigh-Taylor instability for $Re = 256$ (top) and $Re = 2048$ (bottom). Left: Density contours at different normalized times $t.U^*/L = 1, 2, 3, 4, 5$ obtained for the fine mesh. Right: time evolution of the position of both bubble (solid) and spike (dashed). (\square) indicates the coarse mesh, (+) for the fine mesh, and (\circ) for the reference from He et al.⁷³.

208 based on inflow mean injection velocity, source diameter and kinematic viscosity, is 1273.
 209 The specific momentum, M_0 , buoyancy, F_0 , mass, Q_0 , and the Morton length scale, L_M , are
 210 defined as:

$$F_0 = 2\pi g \int_0^\infty U_z \frac{\Delta T}{T} r dr, \quad M_0 = 2\pi \int_0^\infty U_z^2 r dr, \quad Q_0 = 2\pi \int_0^\infty U_z r dr, \quad L_M = \frac{M_0^{3/4}}{F_0^{1/2}} \quad (26)$$

211 where r is the radial coordinate. Morton²⁸ and Morton and Middleton⁸³ introduced the
 212 source parameter Γ_0 that characterizes the plume as being either lazy ($\Gamma_0 > 1$), pure ($\Gamma_0 = 1$)
 213 or forced ($0 < \Gamma_0 < 1$):

$$\Gamma_0 = \frac{5Q_0^2 F_0}{8\sqrt{\pi}\alpha M_0^{5/2}} \quad (27)$$

214 with α the entrainment coefficient explained in details later on. The value of Γ_0 in our

simulation is around 0.9, which indicates a forced plume, having a value of Γ_0 near unity says that the plume is forced but not too much as a result the buoyancy is significant near the source which explains the acceleration zone detailed later.

A. Numerical set-up

The computational domain is a box of size $18D \times 9D \times 9D$. A uniform mesh, composed of $300 \times 150 \times 150$ cells, is considered. The simulation was performed with ProLB on processors. The time-step, based on the sound speed, is $\delta_t = 4.5 \times 10^{-6}$ s. In accordance with previous LES of this configuration⁵⁵, the Vreman turbulence model, described in Sec. IB, is applied with a turbulent Prandtl number of $Pr_t = 0.3$.

The boundary conditions are as follows: at the outlet, a Dirichlet condition is considered for pressure whereas a Neumann condition is applied for other variables with a clip for the axial velocity to prevent any backflow of the plume. Typical inflow/outflow boundary conditions are considered for the vertical sides.

At the inlet, temperature and velocity were imposed to represent a plume source.

For the inlet boundary condition, we followed the strategy of Zhou et al.^{55,84} to ensure a transition from laminar to turbulence at a very short distance of the exit, consistently with the experimental observations of Shabbir and George⁴⁷. This kind of fluctuations work more as perturbations with artificial nature so they are not divergence free. However, this does not represent an important issue because the associated time scale is large compared to the flow turbulent time scales (the fastest time scale of our injection is around 0.2s). As a consequence, the impact of this synthetic injection vanishes few diameters away from the inlet where we start performing our analysis. It consists in superimposing azimuthal disturbances:

$$u'(r) = AU_0(r) \left[\left(1 - \frac{r}{D}\right) \sum_{n=1}^N \sin(2\pi ft/n) + \frac{r}{D} \sum_{n=1}^N \sin(2\pi ft/n + \theta) \right] \quad (28)$$

to a mean flow $U_0(r)$ corresponding to a pipe profile:

$$U_0(r) = \frac{1}{2}U_0 [1 - \tanh(b_2(2r/D - D/2r))]. \quad (29)$$

A is the amplitude of the forcing and $N = 6$ is the number of the modes. f is the frequency of the forcing, that is determined by the jet preferred mode corresponding to a Strouhal

241 number, $St = fD/U_0$, of 0.3, leading to $f = 4.629\text{Hz}$. In the mean pipe flow profile, θ is the
 242 azimuthal angle and $b_2 = 6.25^{85}$.

243 Note that Eq. (28) was slightly modified from the original formulation^{86,87}, which pre-
 244 sented a singularity at the center. The forcing amplitude $A = 0.2/\sqrt{3}$, corresponds to a
 245 RMS fluctuations of 20% for the axial velocity and $A = 0.01/\sqrt{3}$ corresponds to a RMS
 246 fluctuations of 1% for the other two components.

247 The time-averaged statistics (mean, rms,..) presented hereafter were collected over 15
 248 forcing cycles = 20 s once a statistical steady state was reached. The forcing cycle is defined
 249 by the longest period of the sine series in Eq. (28) = 1.3 s.

250 B. Results and discussion

251 1. Qualitative description

252 Figure 6 illustrates the transition process through a snapshot of the three dimensional
 253 iso-surface for the Q-criterion⁸⁸ along with temperature and density fields. The Q-criterion
 254 is defined as:

$$Q = \frac{1}{2}(\|\Omega\|^2 - \|S\|^2), \quad (30)$$

255 where S and Ω are the strain rate and the vorticity tensor, respectively:

$$\Omega = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T), \quad (31)$$

$$S = \frac{1}{2}(\nabla\mathbf{u} - \nabla\mathbf{u}^T), \quad (32)$$

256 The Q-criterion defines the areas where the vorticity magnitude is larger than the mag-
 257 nitude of the strain rate, such that $Q > 0$ indicates the existence of a vortex. The potential
 258 core of the plume becomes rapidly turbulent after few diameters from the source which is
 259 consistent with the experimental observations of Shabbir and George⁴⁷. The transition oc-
 260 curs due to the growth of azimuthal instabilities that forms large coherent energy containing
 261 structures which eventually break down to generate small-scale turbulence.

262 Figure 7 shows the energy spectrum based on the axial velocity at distance $z/D = 4$, it
 263 shows the energy cascading reported by the theory of Kolmogorov⁸⁹ and that we have the

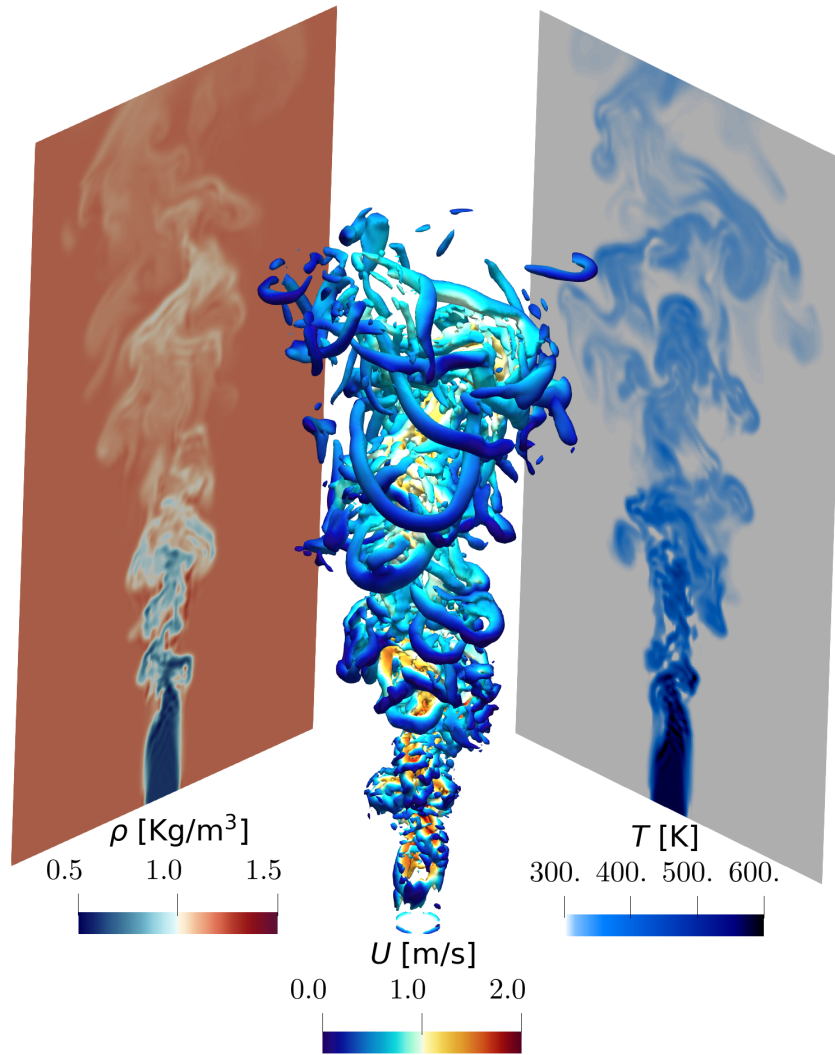


Figure 6: Instantaneous 3D Q-criterion colored by velocity magnitude alongside density and temperature fields

264 correct power law of $-5/3$ in the inertial range, also the dissipation range was detected at
 265 higher frequencies. In addition, in Figure 7 the spectrum for temperature fluctuations is
 266 shown, the spectrum initially shows the $-5/3$ power law in the so called inertial-convection
 267 region. Afterwards, a region is expected where the spectrum decays sharply and follows
 268 a -3 power law, which is a unique characteristic of the forced plumes, and it belongs to

269 the inertial-diffusive subrange proposed by Papanicolaou & List⁴⁶. Kostovinos⁹⁰ argued
 270 experimentally that the slope change from $-5/3$ to -3 is due to strong energy feeding as a
 271 result of the large plume vortices driven by buoyancy force. This region cannot be clearly
 272 identified on the spectrum of temperature fluctuations in Figure 7.

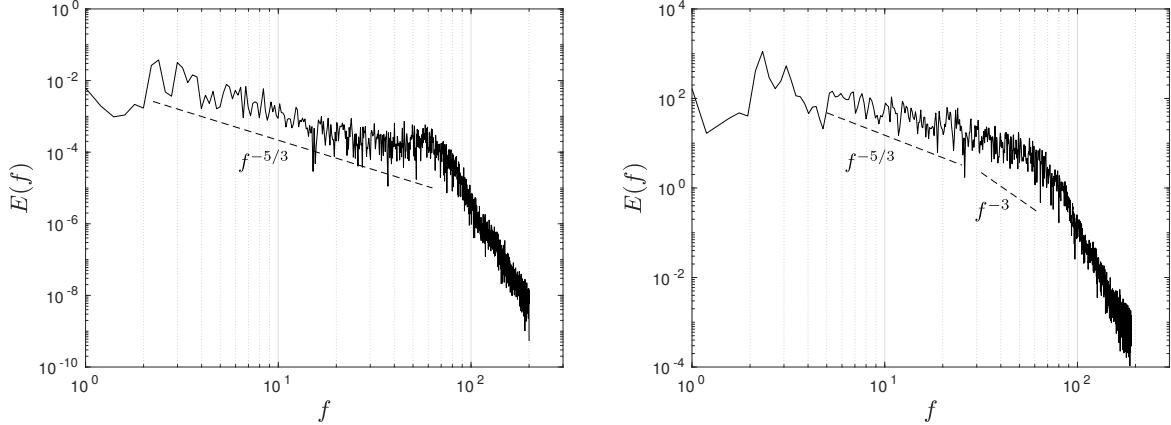


Figure 7: Temporal energy spectrum at $z/D = 4$ for axial velocity (left), temperature
 (right). Dashed lines indicate the expected characteristic slopes.

273

274

275 2. Axial mean quantities

276 Figure 8 compares the centerline time-averaged axial velocity U_c , and temperature T_c , to
 277 the experimental data of Shabbir and George⁴⁷, who proposed the following correlation in
 278 the plume-like region:

$$U_c = A_U z^{-1/3} F_0^{1/3}, \quad \frac{T_a}{T_c} = 1 - A_T z^{-5/3} F_0^{2/3} / g, \quad (33)$$

279 where $A_T = 9.4$ and $A_U = 3.4$ were fitted from the experimental results (see also in Table
 280 II). The centerline velocity in Fig. 8 increases rapidly from its initial value at the inlet to a
 282 maximum value of about 1.8 at $z/D \approx 2.5$ and then decreases afterwards rapidly to reach
 283 values lower than the inflow velocity after about 6 diameters. This behavior was also ob-
 284 served by Lingens et al.⁹¹ who experimentally investigated buoyant jet diffusion flame. The
 285 initial acceleration in the near field is due to the large buoyancy force resulting from large
 286 temperature (density) difference between the plume core and the ambient. The rapid decel-
 287 eration after the peak results from the turbulent mixing of the plume with the surrounding

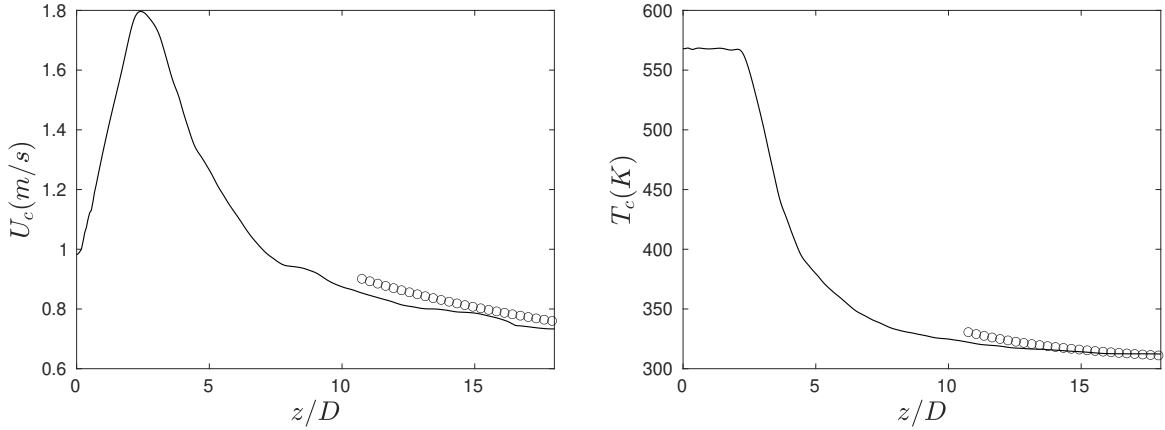


Figure 8: Centerline mean axial velocity (left), and Temperature (right) profiles. Solid line for the simulation, symbols for experimental data of Shabbir and George⁴⁷

fluid, which decreases the temperature. The rapid decrease in temperature downstream the potential core is clearly evidenced in Fig. 8. The location of the transition from jet-like to plume-like behavior can be identified through the rates of decrease which have to scale with $z^{-1/3}$ and $z^{-5/3}$ for velocity and temperature, respectively. The numerical model predicts the transition at $z/D \approx 10-11$ which is consistent with the experiments of Shabbir and Georges⁴⁷ where it was estimated to occur at $z/D = 10.5$. In the plume-like region, the model reproduces quantitatively the evolution of both axial velocity and temperature with z/D , although U_c is on the whole slightly underestimated.

The non-dimensional mean axial velocity $U_c z / \sqrt{M_0}$ is plotted as a function of the non-dimensional axial distance $\xi = z/L_M$ in Fig. 9. The transition to the plume-like region (i.e. the slope change) is predicted around $\xi = 4 \sim 5$ which is consistent with the finding of Morton et al.⁴³ who reported that a forced plume will reach a pure plume behavior for $z/L_M > 5$. In addition, our simulation exhibits a good agreement with the experimental profile obtained from the correlation of Shabbir and George⁴⁷ (see Eq. 33) in the plume-like region.

Forced plumes becomes plume-like far away from the source in homogeneous environment even if the injected momentum flux is large when the function Γ changes from a value smaller than 1 at the source to a value of 1 in the far field. Four regions were identified in the present simulation: 1) a non-buoyant region where momentum dominates the flow, 2) an acceleration region where the plume is accelerated due to gravity, 3) an intermediate

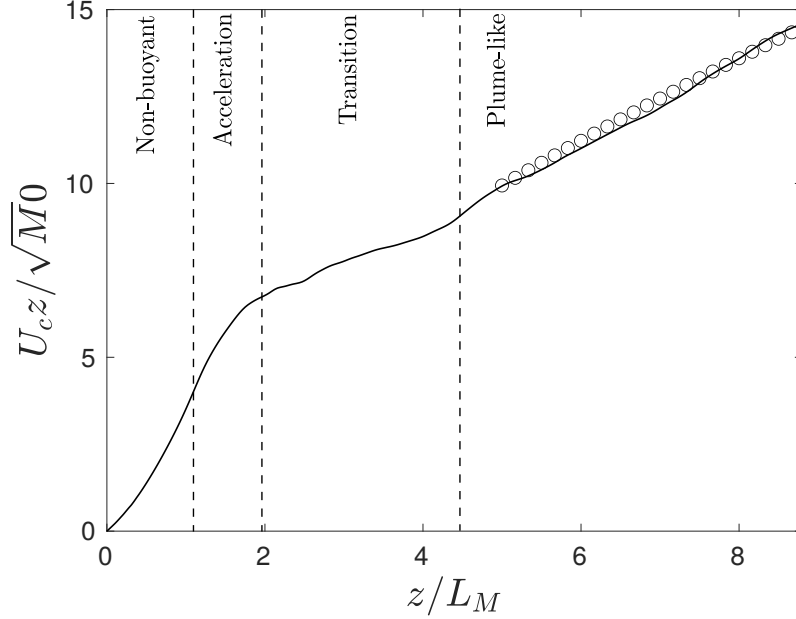


Figure 9: Centerline mean non-dimensional axial velocity profile. Solid line for the simulation and symbols for experiment of Shabbir and George⁴⁷

309 region where influence of initial momentum weakens, and 4) the plume-like region (i.e. self-
 310 similarity region) where the plume dynamics is dominated solely by the buoyancy forces.
 311 This picture is consistent with the descriptions of Gebhart et al.⁹² and Chen and Rodi⁹³
 312 although they did not report the acceleration region (i.e. region 2). Note that the limits of
 313 each region in Fig. 9 are defined using the velocity inflection points, consistently with the
 314 global behavior of the plume.

315 **3. Fluctuations quantities**

316 In this section, the axial evolution of the rms values of axial velocity and temperature
 317 fluctuations and the cross-correlation between velocity and temperature fluctuations are
 318 discussed and compared with experiments^{45–48}, for which the fitting parameters are reported
 319 in Tab. II.

321 Figure 10 presents the rms values of axial velocity and temperature fluctuations. As
 322 expected, the velocity fluctuations are about 20% at vicinity of the inflow plane and corre-
 323 sponds to the imposed disturbance level. The velocity fluctuations decrease in the potential
 324 core region of the plume before starting to increase very abruptly in the laminar to turbu-

Reference	A_T	A_U	B_T	B_U	$\overline{(T'^2)}^{1/2}/\overline{\Delta T_c}$	$\overline{(u'_z)^2}^{1/2}/\overline{U_c}$	$\overline{u'_z T'}/\overline{(u'_z)^2}^{1/2}\overline{(T'^2)}^{1/2}$
Shabbir & George ⁴⁷	9.4	3.4	68	58	0.4	0.33	0.67
George et al. ⁴⁵	9.1	3.4	65	55	0.38	0.28	0.67
Papanicolaou & List ⁴⁶	14.28	3.85	80	90	0.42	0.25	0.51
Nakagome & Hirata ⁴⁸	11.5	3.89	48.1	63	0.36	0.25	0.46

Table II: Summary of mean flow parameters and turbulence intensities for different experiments

lence transition region, the initial drop in velocity fluctuations is due to the artificial nature of the fluctuations imposed at the inlet. These artificial fluctuations, without a proper cascade, are dissipated very quickly; however, they constitute the seed for a correct transition to turbulence with a realistic energy cascade in the far field where we perform our analysis. In the plume-like region, both velocity and temperature fluctuations decrease at a same rate as mean velocity and temperature to ensure constant ratio of $\overline{u'^2}^{1/2}/U_c$ and $\overline{T'^2}^{1/2}/(T_c - T_a)$. The predicted velocity-based turbulence intensity in the plume-like region is lower than those of 0.28 and 0.33 reported by George et al.⁴⁵ and Shabbir and George⁴⁷, respectively. It is in better agreement with those of 0.25 reported by Papanicolaou and List⁴⁶ and Nakagome and Hirata⁴⁸. On the other hand, Fig. 10 shows that the temperature-based turbulence intensity is also consistent with the available data.

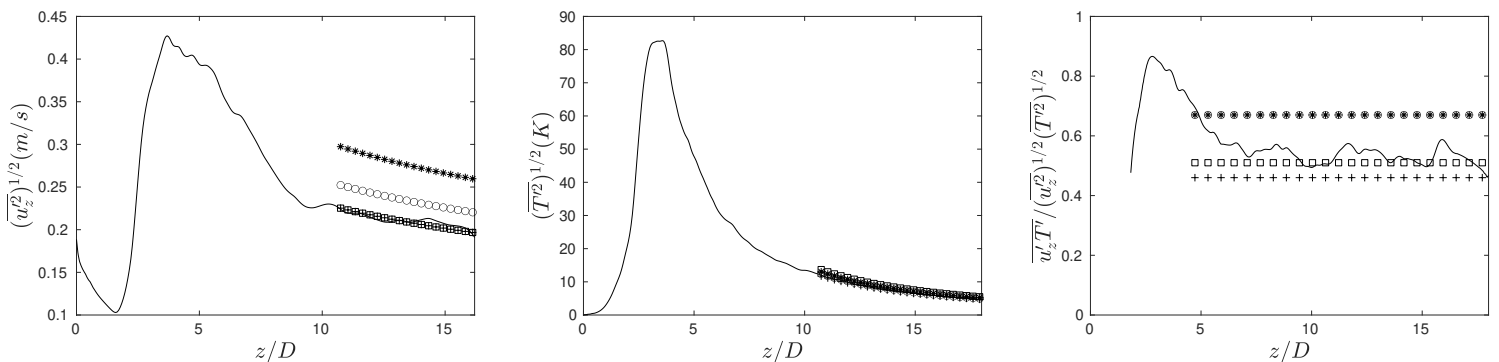


Figure 10: Center line profiles of r.m.s of axial velocity (left), temperature (center), and the cross-correlation of velocity and temperature fluctuations (right). Solid line for simulation, (*) for Shabbir & George⁴⁷, (o) for George et al.⁴⁵, (□) for Papanicolaou & List⁴⁶, and (+) for Nakagome & Hirata⁴⁸.

336 Figure 10 shows the evolution of the cross correlation between velocity and temperature
337 fluctuations, $\overline{u'T'}/(\overline{(u'^2)})^{1/2}(\overline{(T'^2)})^{1/2}$, along the center line. It can be clearly observed that
338 velocity and temperature fields are positively correlated in this type of flows with a predicted
339 nearly constant value in plume-like region of about 0.55. This value is lower than those
340 reported by George and co-workers^{45,47} in the range 0.6-0.7, averaged to 0.67 (see Table II),
341 and in closer agreement with those of 0.46 and 0.51 reported by Nakagome and Hirata⁴⁸ and
342 Papanicolaou and List⁴⁶, respectively.

343 4. *Self-similarity*

344 An important feature of the mean flow in the fully-developed region of turbulent posi-
345 tively buoyant plumes is the “self-similarity” or “self-preserving” behaviour. The radial mean
346 velocity and temperature profiles follow a Gaussian shape and become wider as the plume
347 rises. The profiles collapse on the same curve when considering appropriate dimensionless
348 variables:

$$\frac{U_z}{U_c} = \exp\left\{-B_u \frac{r^2}{z^2}\right\}, \quad \frac{T - T_a}{T_c - T_a} = \exp\left\{-B_T \frac{r^2}{z^2}\right\} \quad (34)$$

349 The coefficients B_u and B_T are unknown empirical constants that can be obtained by
350 assuming a linear growth of the plume width b ⁴³:

$$\frac{b}{z} = \frac{6}{5}\alpha = \text{const}, \quad (35)$$

351 The coefficients will then be calculated using $B_u = \sqrt{z/b_u}$ and $B_T = \sqrt{z/b_T}$, where b_u
352 and b_T are the plume width defined by the distance from the centerline to the point at which
353 we have $1/e$ of the centerline values of velocity and temperature, respectively. George et
354 al.⁴⁵ determined by experiments those coefficients as $B_u = 55$ and $B_T = 65$.

355 The radial profiles of mean velocity and temperature from our LES at $z/D = 10, 12, 14, 16$
356 and the profiles of George et al.⁴⁵ form are plotted in Fig. 11. The velocity and the
357 temperature rise above the ambient are normalized by the centreline value. The profiles
358 are plotted versus the non-dimensional radial coordinate $r/(z + z_0)$ where z_0 is the virtual
359 origin of the plume. Empirical relationships were reported to estimate the location of the
360 virtual origin⁵⁵. As pointed out by Yang⁵⁶, the location of virtual origin predicted in the
361 simulation can be different from that estimated by empirical formula. Indeed, this location

362 is significantly affected by the transition from laminar to turbulent whose the prediction is
 363 a difficult task in LES mainly due to its sensitivity to the plume's source inflow condition.
 364 In the present study, the virtual origin was estimated to collapse the radial profiles in the
 365 fully developed region to a single dimensionless Gaussian profile following the methodology
 366 proposed by Yan⁵⁶, giving z_0 set equal to $2.3D$. It can be observed in Fig. 11 that the
 367 self-similarity is well preserved in the simulation and the predicted self-similarity profiles
 368 agree well with those reported by Georges et al.⁴⁵.

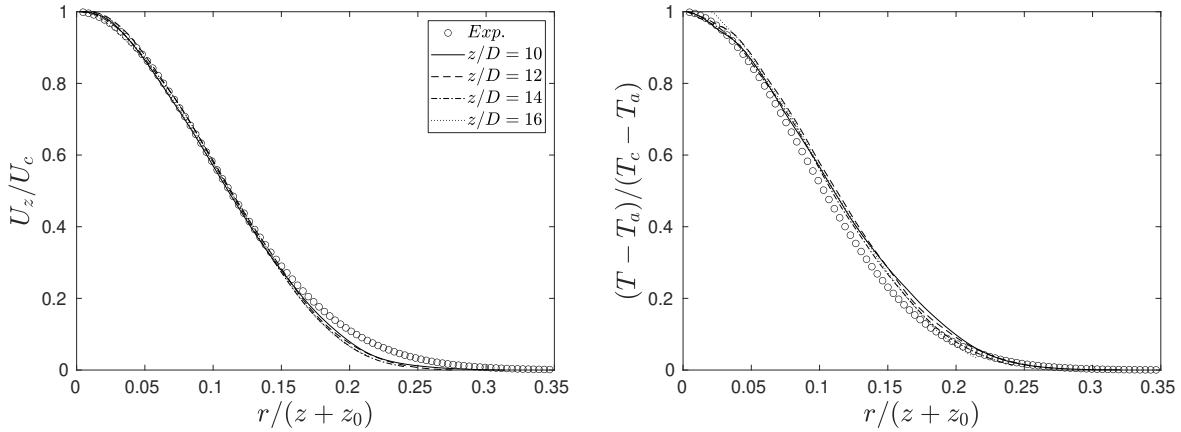


Figure 11: Radial profiles of mean axial velocity (left) ,and mean temperature (right) at four axial positions compared to the experiments of George et al.⁴⁵

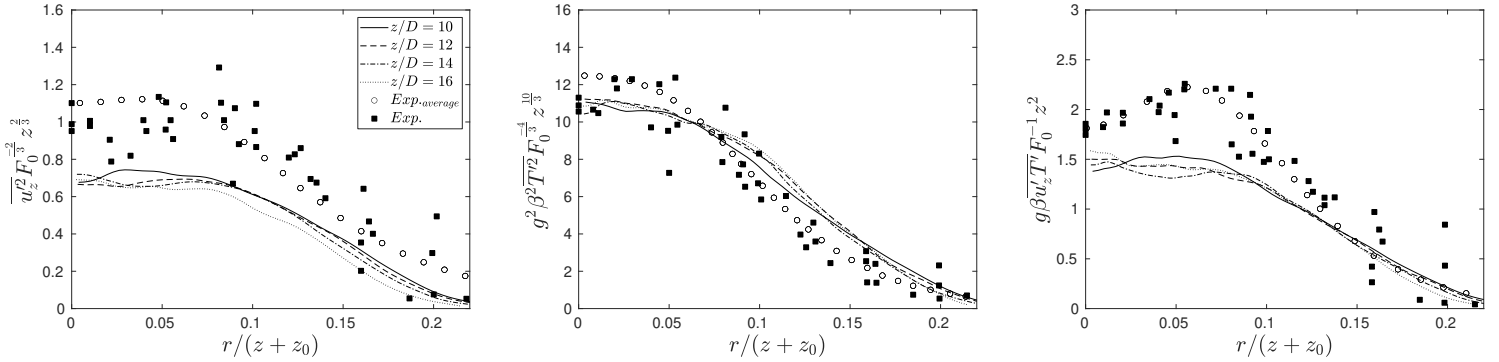


Figure 12: Radial profiles at $z/D = 10, 12, 14, 16$ for normalized r.m.s of axial velocity fluctuation (left), r.m.s of temperature fluctuations (middle), and cross correlation of both velocity and temperature fluctuations (right).

369 Following Shabbir & George⁴⁷, the radial profiles of r.m.s values of axial velocity and
 370 temperature and of the cross correlation between velocity and temperature fluctuations are

371 plotted in terms of the similarity variables in Fig. 12. The predicted profiles clearly exhibit
 372 a self-similar behavior. The agreement with the experimental data is reasonable although,
 373 consistently with Fig. 10, both r.m.s values of axial velocity fluctuations and the cross
 374 correlation between velocity and temperature fluctuations are overall underestimated.

375 5. *Entrainment*

376 The mechanism of turbulent mixing which brings air into the buoyant plume is called
 377 entrainment. The ideal plume theory is based on both Boussinesq and top-hat radial-profile
 378 assumptions and assumes that the mean entrained flux across the edge of the plume E
 379 (entrainment rate) is proportional to the local upward velocity W . An air entrainment
 380 coefficient is then defined as:

$$\alpha = \frac{E}{bW} \quad (36)$$

381 where E , W , b are known as the top-hat variables of entrainment rate, local vertical
 382 velocity and plume width defined by Turner⁹⁴:

$$b^2W = \int_0^\infty U_z r dr, \quad b^2W^2 = \int_0^\infty U_z^2 r dr, \quad E = \frac{d}{dz} \left(\int_0^\infty U_z r dr \right) \quad (37)$$

383 The Plume width, b , can be calculated as the value at which velocity or temperature
 384 reaches a value of $1/e$ of the centerline value as indicated by Morton et al.⁴³. This will be
 385 referred to as (*method 1*) hereafter. It can be also obtained from Eq. 37, as $b^2W/\sqrt{b^2W^2}$.
 386 This second method will be referred to as (*method 2*) hereafter. Figure 13 compares the two
 387 methods. The experimental slope obtained by George et al.⁴⁵ and the numerical prediction
 388 obtained by Zhou et al.⁵⁵ are also plotted in Fig. 13. Both the present predicted velocity
 389 and temperature half-widths decrease first due to the "necking" process in the near field,
 390 as observed experimentally by Cetegen⁹⁵, before, as expected, increasing almost linearly in
 391 plume region. The two methods provide on the whole consistent predictions that agree with
 392 both the experimental slope and the numerical results obtained by Zhou et al.⁵⁵.

393 The entrainment coefficient, α , can be calculated using Eq. 35. This method requires
 394 the knowledge of the width of b , along the plume axis. It can be obtained either from tem-
 395 perature and velocity radial profiles (*method 1*) or from Eq. 37 (*method 2*), as discussed
 396 previously. Another method was adopted by Zhou et al.⁵⁵ from Eqs. 36 and 37, leading to

397 $\alpha = E/\sqrt{b^2W^2}$. This method will be referred to as (*method 3*). Figure 13 shows that the
 398 three methods provide consistent results in the far-field. Our results agrees well with the
 399 LES of Zhou et al.⁵⁵ which settles on a constant value in the far-field, $\alpha = 0.09 - 0.1$. Our
 400 predictions of α in the plume region are also close to the value of 0.116 adopted by Morton
 401 in his plume model²⁸ and the experimental value 0.108 reported by George et al.⁴⁵.

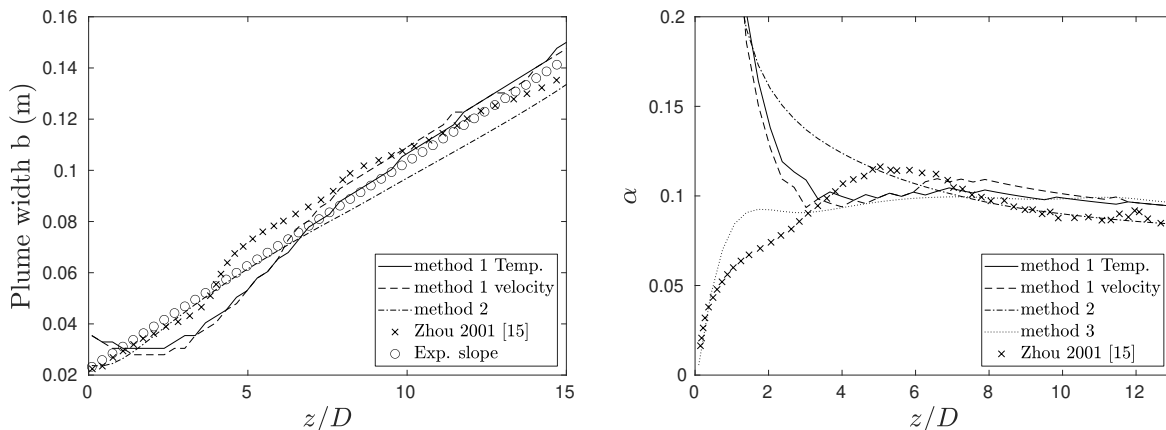


Figure 13: Evolution with the height of (left) the plume width and (right) the entrainment coefficient α

402 Integrating radially the momentum and energy equations across the flow introduces two
 403 fundamental quantities⁴⁷. The first is the momentum flux, M that can be normalized by
 404 the inflow momentum flux, M_0 (see Table I):

$$M = 2\pi \int_0^\infty (U_z^2 + \overline{u_z'^2} - \overline{v'^2}) r dr \quad (38)$$

405 The moment flux ratio increases with the height according to the following relationship⁹⁶:

$$\frac{M}{M_0} = k \left(\frac{x}{L_M} \right)^{4/3} \quad (39)$$

406 Different values of 0.35⁹⁶, 0.34⁴⁷ and 0.29⁴⁶ were reported for the coefficient k . Fig. 14
 407 compares our result to these experimental results. Model predictions are in good agree-
 408 ment with the experiments of Shabbir and George⁴⁷ and Fisher⁹⁶ but overpredict that of
 409 Papanicolaou and List⁴⁶.

410 The second is the buoyancy flux F , that has to be conserved along the plume

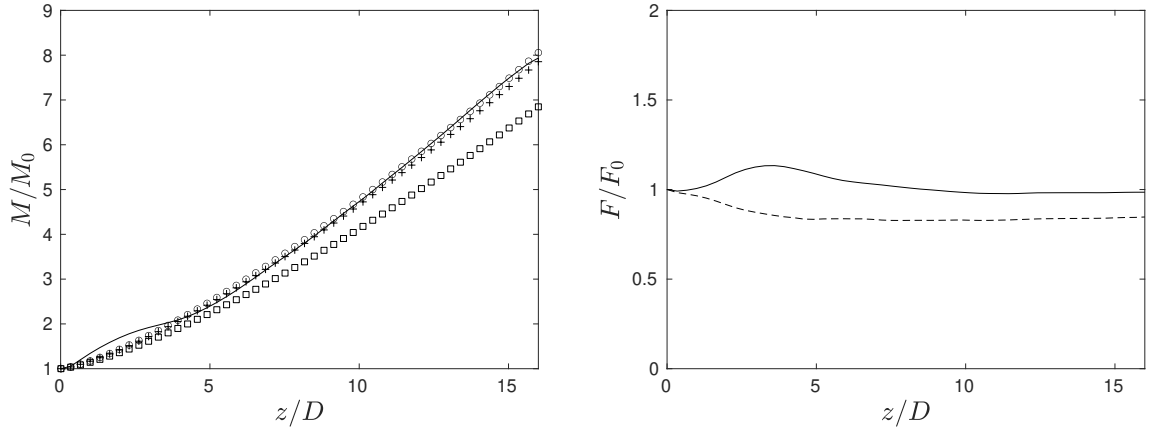


Figure 14: Axial profile of momentum flux ratio (left). The solid line represents the present LES, whereas the symbols represent the experimental data of Fischer et al.⁹⁶ (o), (+) for Shabbir & George⁴⁷ and (□) for Papanicolaou & List⁴⁶. Axial profile of buoyancy flux ratio (right), solid line includes the turbulent heat flux while dash line does not.

411 height:

$$F = 2\pi g \int_0^\infty \left(U_z \frac{\Delta T}{T} + \frac{\overline{u'_z T'}}{T} \right) r dr \quad (40)$$

412 The buoyancy flux is normalized by its injection value, F_0 . Figure 14 shows the evolution
 413 of F/F_0 along the plume height. The simulated normalized buoyancy flux evolves around
 414 unity, consistently with the theory (solid line). It appears clearly by comparing the solid
 415 and dashed lines that the turbulent contribution is essential. When it is disregarded, the
 416 buoyancy flux decreases with the axial distance and is no more conserved. The turbulence
 417 contribution is predicted around 15% – 20% as also noted by Shabbir & George⁴⁷, while
 418 George et al.⁴⁵ and Papanicolaou & List⁴⁶ found the contribution to be about 15%.

419 IV. CONCLUDING REMARKS

420 A recursive regularized pressure based LBM solver (ProLB) was tested for buoyancy
 421 driven flows.

422

423 The solver was able to correctly validate the Rayleigh Bénard cavity test case for dif-
 424 ferent Rayleigh numbers $Ra = 10^4, 10^5, 10^6$, vertical and horizontal velocity profiles as well

425 as Nusslet number profiles at the bottom wall were all in a good agreement with the reference.

426

427 As for the Rayleigh Taylor test case, we were able to correctly predict the instantane-
428 neous evolution of the positions of bubble and spike for two different Reynolds numbers
429 $Re = 256, 2048$. In addition, the test case was run on a coarser mesh to test the robustness
430 of the solver and the results were abundantly satisfying.

431

432 For the 3d forced plume simulation, which is a critical test case in which the buoyancy is
433 highly coupled with momentum and turbulent mixing, the solver was able to anticipate the
434 correct physics of a thermal plume from numerous aspects listed below:

- 435 • The velocity energy spectrum follows the Kolmogorov theoretical slope of $-5/3$ indi-
436 cating a proper resolution of the turbulence energy cascading as reported in the
437 literature.
- 438 • Axial profiles of mean velocity and temperature were in a good agreement with the
439 experimental data.
- 440 • Our forced-plume reaches a plume-like region at around $z/L_m = 4 \approx 5$ which is
441 consistent with the findings in the literature.
- 442 • The axial profiles of rms for velocity and temperature also were in a good agreement
443 with the experiments, we should emphasize that we did not take into account the
444 experimental errors which are significant specially for the second order statistics.
- 445 • The cross-correlation between velocity and temperature has a high positive value which
446 compares well with the reported values from experiments and indicates a strong cou-
447 pling between the velocity and temperature fluctuations due to gravity.
- 448 • Self similarity profiles in the far field (i.e. plume-like region) were achieved for both
449 mean and rms of velocity and temperature.
- 450 • The growth rate of the plume was examined through the spatial evolution of the plume
451 width. The growth of the plume compared very well with experimental and numerical
452 references.

- 453 • The entrainment of fluid from the surrounding was correctly predicted by examining
454 the entrainment coefficient α , and the predictions were in a good agreement with the
455 theoretical, experimental and numerical references.
- 456 • Integral quantities, mainly Buoyancy flux and momentum flux, were compared with
457 the experiments and both were in a good agreement, we emphasize about the finding
458 that the turbulent heat flux participates by around 20% in the total buoyancy flux
459 which is consistent with the experiments.

460 From all the previous points we can conclude that our solver is capable of reproducing the
461 physics of a thermal plume correctly whether the mean values, the second order statistics or
462 even integral quantities through the plume, and that our code can handle any type of flows
463 with variable densities regardless of their complexity.

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467 formance computing resources.

468 DATA AVAILABILITY

469 The data that support the findings of this study are available from the corresponding
470 author upon reasonable request.

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692 **Appendix A: Expressions for the LBM solver**

In regularized LBM, distribution functions will be constructed using an orthogonal poly-
nomial basis. The basis of the D3Q19r lattice used in the current study consists of 19

polynomials, read¹⁷

$$\mathcal{H}_i^{(0)} \equiv 1, \quad \mathcal{H}_{i,\alpha}^{(1)} \equiv c_{i\alpha}, \quad \mathcal{H}_{i,\alpha\beta}^{(2)} \equiv c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta}, \quad (\text{A1})$$

$$\mathcal{H}_{i,1}^{(3r)} \equiv \mathcal{H}_{i,xy}^{(3)} + \mathcal{H}_{i,yzz}^{(3)}, \quad (\text{A2})$$

$$\mathcal{H}_{i,2}^{(3r)} \equiv \mathcal{H}_{i,xzz}^{(3)} + \mathcal{H}_{i,xyy}^{(3)}, \quad (\text{A3})$$

$$\mathcal{H}_{i,3}^{(3r)} \equiv \mathcal{H}_{i,yyz}^{(3)} + \mathcal{H}_{i,xxz}^{(3)}, \quad (\text{A4})$$

$$\mathcal{H}_{i,4}^{(3r)} \equiv \mathcal{H}_{i,xy}^{(3)} - \mathcal{H}_{i,yzz}^{(3)}, \quad (\text{A5})$$

$$\mathcal{H}_{i,5}^{(3r)} \equiv \mathcal{H}_{i,xzz}^{(3)} - \mathcal{H}_{i,xyy}^{(3)}, \quad (\text{A6})$$

$$\mathcal{H}_{i,6}^{(3r)} \equiv \mathcal{H}_{i,yyz}^{(3)} - \mathcal{H}_{i,xxz}^{(3)}, \quad (\text{A7})$$

$$\mathcal{H}_{i,1}^{(4r)} \equiv \frac{4}{9} \left(3 + 2\sqrt{3} \right) \mathcal{D}_{i,xyz}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,xzy}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,zyx}^{(4)}, \quad (\text{A8})$$

$$\mathcal{H}_{i,2}^{(4r)} \equiv \frac{4}{9} \left(3 + 2\sqrt{3} \right) \mathcal{D}_{i,xzy}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,xyz}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,zyx}^{(4)}, \quad (\text{A9})$$

$$\mathcal{H}_{i,3}^{(4r)} \equiv \frac{4}{9} \left(3 + 2\sqrt{3} \right) \mathcal{D}_{i,zyx}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,xzy}^{(4)} + \frac{4}{9} \left(3 - \sqrt{3} \right) \mathcal{D}_{i,xyz}^{(4)}, \quad (\text{A10})$$

where

$$\mathcal{H}_{i,\alpha\beta\gamma}^{(3)} \equiv c_{i\alpha}c_{i\beta}c_{i\gamma} - c_s^2[c_{i\alpha}\delta_{\beta\gamma} + c_{i\beta}\delta_{\gamma\alpha} + c_{i\gamma}\delta_{\alpha\beta}], \quad (\text{A11})$$

$$\mathcal{D}_{i,\alpha\beta\gamma}^{(4)} \equiv \mathcal{H}_{i,\alpha\alpha\beta\beta}^{(4)} + \frac{c_s^2}{2} \mathcal{H}_{i,\gamma\gamma}^{(2)}, \quad (\text{A12})$$

$$\begin{aligned} \mathcal{H}_{i,\alpha\beta\gamma\delta}^{(4)} &\equiv c_{i\alpha}c_{i\beta}c_{i\gamma}c_{i\delta} + c_s^4(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\beta\gamma}\delta_{\delta\alpha} + \delta_{\delta\alpha}\delta_{\beta\gamma}) \\ &\quad - c_s^2(c_{i\alpha}c_{i\beta}\delta_{\gamma\delta} + c_{i\beta}c_{i\gamma}\delta_{\delta\alpha} + c_{i\gamma}c_{i\delta}\delta_{\alpha\beta} + c_{i\delta}c_{i\alpha}\delta_{\beta\gamma} + c_{i\gamma}c_{i\alpha}\delta_{\beta\delta} + c_{i\beta}c_{i\delta}\delta_{\alpha\gamma}). \end{aligned} \quad (\text{A13})$$

693 Any distribution function in the D3Q19r lattice can be written as a (weighted) sum of
694 the contributions from each base polynomial. For instance, the equilibrium distribution in
695 equation (14) reads

$$f_i^{\text{eq},19r} = \omega_i \left\{ a^{(0),\text{eq}} + \frac{\mathcal{H}_{i,\alpha}^{(1)}}{c_s^2} a_\alpha^{(1),\text{eq}} + \frac{\mathcal{H}_{i,\alpha\beta}^{(2)}}{2c_s^4} a_{\alpha\beta}^{(2),\text{eq}} + \frac{\mathcal{H}_{i,\gamma}^{(3r)}}{6c_s^6} a_\gamma^{(3r),\text{eq}} + \frac{\mathcal{H}_{i,\delta}^{(4r)}}{24c_s^8} a_\delta^{(4r),\text{eq}} \right\}, \quad (\text{A14})$$

where

$$a^{(0),\text{eq}} = \rho\theta, \quad a_\alpha^{(1),\text{eq}} = \rho u_\alpha, \quad a_{\alpha\beta}^{(2),\text{eq}} = \rho u_\alpha u_\beta \quad (\text{A15})$$

$$a_1^{(3r),\text{eq}} = 3(\rho u_x u_x u_y + \rho u_y u_z u_z), \quad (\text{A16})$$

$$a_2^{(3r),\text{eq}} = 3(\rho u_x u_z u_z + \rho u_x u_y u_y), \quad (\text{A17})$$

$$a_3^{(3r),\text{eq}} = 3(\rho u_y u_y u_z + \rho u_x u_x u_z), \quad (\text{A18})$$

$$a_4^{(3r),\text{eq}} = \rho u_x u_x u_y - \rho u_y u_z u_z, \quad (\text{A19})$$

$$a_5^{(3r),\text{eq}} = \rho u_x u_z u_z - \rho u_x u_y u_y, \quad (\text{A20})$$

$$a_6^{(3r),\text{eq}} = \rho u_y u_y u_z - \rho u_x u_x u_z, \quad (\text{A21})$$

$$a_1^{(4r),\text{eq}} = -\rho c_s^2 \left[\frac{-4\sqrt{3}-6}{9} u_z^2 + \frac{2\sqrt{3}-6}{9} (u_x^2 + u_y^2) \right], \quad (\text{A22})$$

$$a_2^{(4r),\text{eq}} = -\rho c_s^2 \left[\frac{-4\sqrt{3}-6}{9} u_y^2 + \frac{2\sqrt{3}-6}{9} (u_x^2 + u_z^2) \right], \quad (\text{A23})$$

$$a_3^{(4r),\text{eq}} = -\rho c_s^2 \left[\frac{-4\sqrt{3}-6}{9} u_x^2 + \frac{2\sqrt{3}-6}{9} (u_y^2 + u_z^2) \right]. \quad (\text{A24})$$

696 It is worth noting that the the forth-order coefficients ($a^{(4),\text{eq}}$) are added to improve
 697 the isotropicity of the lattice, which could be quite important considering the round jet
 698 simulation in the current study.

699 The third-order off-equilibrium terms are reconstructed recursively from the second-order
 700 non-equilibrium tensor as

$$\begin{aligned} a_{\alpha\beta\gamma}^{(3),\text{neq}} &= u_\alpha a_{\beta\gamma}^{(2),\text{neq}} + u_\beta a_{\alpha\gamma}^{(2),\text{neq}} + u_\gamma a_{\alpha\beta}^{(2),\text{neq}} \\ a_1^{(3r),\text{neq}} &\equiv a_{xxy}^{(3),\text{neq}} + a_{yzz}^{(3),\text{neq}} \\ a_2^{(3r),\text{neq}} &\equiv a_{xzz}^{(3),\text{neq}} + a_{xyy}^{(3),\text{neq}} \\ a_3^{(3r),\text{neq}} &\equiv a_{yyz}^{(3),\text{neq}} + a_{xxz}^{(3),\text{neq}} \\ a_4^{(3r),\text{neq}} &\equiv a_{xxy}^{(3),\text{neq}} - a_{yzz}^{(3),\text{neq}} \\ a_5^{(3r),\text{neq}} &\equiv a_{xzz}^{(3),\text{neq}} - a_{xyy}^{(3),\text{neq}} \\ a_6^{(3r),\text{neq}} &\equiv a_{yyz}^{(3),\text{neq}} - a_{xxz}^{(3),\text{neq}} \end{aligned} \quad (\text{A25})$$

701 Depending on the order of the Gauss-Hermite quadrature⁶⁷ used in the LB model, an
 702 adequate forcing term should be added to achieve a correct viscous stress tensor:

$$a_{\alpha\beta}^{\text{neq}} \approx -\Pi_{\alpha\beta} = -\mu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{D} \frac{\partial u_\gamma}{\partial x_\gamma} \delta_{\alpha\beta} \right), \quad (\text{A26})$$

703 with D the spatial dimension. For the D3Q19r basis, the projected forcing term reads as

$$a_{\alpha\beta}^{FE} = c_s^2 u_\alpha \left[\frac{\partial(\rho(1-\theta))}{\partial x_\beta} \right] + c_s^2 u_\beta \left[\frac{\partial(\rho(1-\theta))}{\partial x_\alpha} \right] + \delta_{\alpha\beta} \rho c_s^2 \frac{2}{D} \frac{\partial u_\gamma}{\partial x_\gamma} - a_{\alpha\beta}^{\text{cor}} + a_{\alpha\beta}^{FD} \quad (\text{A27})$$

704 where $a_{\alpha\beta}^{\text{cor}}$ is a correction tensor due to the deflection of second order moments of the
705 population introduced by the modification of the mass equation, which can be evaluated as

$$a_{\alpha\beta}^{\text{cor}} \equiv c_s^2 \delta_{\alpha\beta} \frac{\partial(\rho(1-\theta))}{\partial t}, \quad (\text{A28})$$

706 which can be discretized using a backward Euler operator and $a_{\alpha\beta}^{FD}$ the correction tensor due
707 to the defect of the lattice at third order

$$a_{\alpha\beta}^{FD} = - \begin{pmatrix} (\rho u_x^3)_{,x} & (\rho u_x u_y u_z)_{,z} & (\rho u_x u_y u_z)_{,y} \\ (\rho u_x u_y u_z)_{,z} & (\rho u_y^3)_{,y} & (\rho u_x u_y u_z)_{,x} \\ (\rho u_x u_y u_z)_{,y} & (\rho u_x u_y u_z)_{,x} & (\rho u_z^3)_{,z} \end{pmatrix} \quad (\text{A29})$$

708 where all the differential operations are performed using first order upwind FD except for
709 the divergence operator for which a second order centered FD scheme was employed. The
710 final expression of the forcing term is then

$$F_i^E = \frac{\omega_i}{2c_s^4} \mathcal{H}_{i,\alpha\beta}^{(2)} a_{\alpha\beta}^{FE} + F_i^g, \quad (\text{A30})$$

711 where F_i^g is the gravity force term defined as

$$F_i^g = \omega_i \left[\frac{\rho g_\alpha \mathcal{H}_{i,\alpha}^{(1)}}{c_s^2} + \frac{(\rho u_\alpha g_\beta + \rho u_\beta g_\alpha) \mathcal{H}_{i,\alpha\beta}^{(2)}}{2c_s^4} \right], \quad (\text{A31})$$

712 where g_α is the gravity acceleration in the direction α .