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A comparison of different CFD and Gaussian dispersion models

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Abstract

In this paper we investigate different numerical techniques to approximate and model gas dispersion, with a primary focus on modelling the buoyancy effects of dense gasses. We compare the popular Gaussian dispersion model with three different computational fluid dynamics (CFD) models. The three CFD models vary based on complexity and hence the associated computational expense. These include an incompressible flow solver with scalar species transport, an incompressible flow solver with an approximation of the gravitational body force, and a fully compressible, combustion CFD model.

The fully compressible, combustion model used in this paper is the OpenFOAM solver *rhoReactingBuoyantFoam*, where the other two incompressible dispersion models are based on modifications of *pimpleFoam,* a transient, incompressible OpenFOAM solver.

The four dispersion models are compared using Trial 26, of the Thorney Island gas dispersion experiments.

Our results confirm that the Gaussian dispersion model is ill-suited to near field gas dispersion modelling in the presence of obstacles. Similarly, incompressible flow with scalar specie transport, is capable of order of magnitude approximations, and therefore may prove useful for scenario planning when multiple gas-leak scenarios are to be investigated. However, if the density ratio is large, and accuracy is important, our results suggest that a compressible gas dispersion solver is necessary, for which *rhoReactingBuoyantFoam* appears to be a suitable candidate.

Keywords: dense gas dispersion, OpenFOAM, CFD, Gaussian plume

1. Introduction

The accidental release of flammable or toxic gases is a serious health and environmental concern, with potentially deadly consequences. The numerical modelling of gas dispersion offers a powerful means by which to predict the flow and concentration of a gas leak given atmospheric and environmental conditions. Potential risks associated with a gas leak can be better understood by modelling multiple gas leak scenarios. This understanding can also aid in the design of effective early gas leak detection systems or an integrated chemical plant design.

To numerically study the effect of varying gas leak location, intensity and changing environmental factors requires a large set of gas dispersion simulations. Generating the large database of simulations can be a computationally expensive exercise depending on the required model fidelity or complexity. In this paper we compare four gas dispersion modelling techniques with varying complexity.

The most commonly used gas dispersion model is the Gaussian dispersion model [1], where the air pollutant is assumed to have a normal probability distribution. Gaussian dispersion models are capable of modelling continuous, buoyant air pollution while taking wind direction and elevation into account. These models are however limited to flat and smooth topography, limiting the range of their applicability.

On the other end of the computational cost scale, are high-fidelity computational fluid dynamics (CFD) tools. Most advanced CFD solvers can solve for buoyancy effects by accounting for different densities of the gas and atmosphere, the effects of temperature, complex wind patterns, include chemical reactions and provide a choice of several turbulence closure models. While high-fidelity CFD can be used to model a broad variety of complex physics, it assumes a strong interaction between the gas dispersion and the fluid flow. Examples where such a relationship is expected includes the simulation of chemical reactions and combustion [2], the rapid expansion of a pressurised gas [3], and to a lesser extent, flow with varying densities [4, 5].

In the large majority of gas dispersion problems, the gas or pollutant will not influence the outside atmosphere and wind flow. In such cases, it is entirely valid to treat gas dispersion as a scalar transport problem. In so doing, the gas dispersion can be modelled by seeding a source into a pre-computed fluid flow field, and solving a set of scalar transport equations. The simplified model can still account for complex geometries, turbulent flow and complex boundary conditions. Because the air flow and gas transport can be solved separately, incompressible scalar transport is ideal when many different gas release scenarios are to be modelled.

As a final option for gas dispersion modelling, we compare to a mildly compressible flow solution, in the spirit of a Boussinesq approximation. The Boussinesq approximation was introduced [6] to model bouncy driven flow for minor density differences. The approximation assumes fluid flow to be incompressible (constant density) where the effects of density differences only enter in the gravity body force term within the momentum equation. The benefit of a such solution scheme is that we are capable of approximating mild density differences between different gases, while continuing to leverage efficient incompressible fluid flow solvers.

In this study we use OpenFOAM [7], an open-source, finite-volume, modelling toolkit, to compare the three CFD variants. The fully compressible, gas dispersion CFD analysis is computed using the *rhoReactingBuoyantFoam* solver, where the incompressible scalar gas dispersion, and mildly compressible Boussinesq like approximation are both implemented by modifying an existing OpenFOAM transient, incompressible flow solver.

We aim to compare the accuracy of the different gas dispersion models using a heavy gas dispersion test problem which contains an obstacle.

2. Gas dispersion model

2.1. Gaussian plume dispersion model

The Gaussian dispersion model, despite its comparative simplicity, arguably remains the most widely used pollutant dispersion model. The Gaussian dispersion model assumes that the air pollutant dispersion follows a normal Gaussian distribution, which has been extensively validated [8,9].

Assuming a continuous pollutant release, under steady state conditions, the contaminant concentration, $C(x, y, z)$, as a function of the downwind position, (x, y, z), of the source is defined as

$$C(x,y,z) = \frac{Q}{2\pi v \sigma_y \sigma\_z} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-h_z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+h_z}{\sigma_z}\right)^2\right]\right\}, \quad (1)$$

Where Q is the mass emission rate, h the effective height of the contaminant source and, v, the wind speed at the "effective" height. σ_y represents the standard deviation based on cross-wind distribution and σ_z represents the standard deviation based on vertical distribution, both of which have been parametrised based on extensive studies of air stability (turbulence) and distance from the source [8]. To ensure conservation, the ground is considered as a "virtual" reflection source.

2.2. Incompressible flow with scalar transport

Despite their popularity, dispersion models such as Gaussian plume models are unable to account for complex topography or the presence of obstacles. These types of flow problems are better suited to computational fluid dynamics (CFD) [5,10].

In this section we outline the simplest of CFD dispersion models, which is based on standard incompressible flow with passive scalar transport. The release and dispersion of a gas can be described, without reactions, through the prediction of the local mass fraction of each species through the solution of a convection-diffusion equation.

The scalar convection-diffusion equation does influence the fluid flow equations. The scalar transport will therefore not be able to account for any density differences, which may arise either due to gasses of different weights, or thermal buoyancy. Having said that, the benefit of a passive scalar transport description is that the fluid flow solution and scalar transport can be completely decoupled. Multiple gas release scenarios, for different release conditions and locations, can then be modelled using the same precomputed flow field. This can be useful when performing scenario and risk planning, or when creating the observations for a surrogate or reduced order model.

The equation for conservation of mass, or continuity equation, can be written as

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) \quad (2)$$

where ρ is the fluid density and $\boldsymbol{u}$ the flow velocity. For an incompressible fluid, with constant density, the continuity equation reduces to

$$\nabla \cdot \boldsymbol{u} = 0. \quad (3)$$

The conservation of momentum for an incompressible Newtonian fluid can be written as

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \boldsymbol{u}\,, \quad (4)$$

where ν is the fluid's kinematic viscosity.

The local mass fraction for a given species, Y_i, can be predicted given the scalar transport conservation equation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \boldsymbol{u} Y_i) = \nabla \cdot \boldsymbol{J}_i + S_i + R_i, \quad (5)$$

Where $\boldsymbol{J}_i$ is the diffusive flux for species i, S_i represents any source term for the ith species and R_i represents the net rate of production due to chemical reactions. For the purposes of this paper we assume there are no chemical reactions, and therefore set the rate of chemical reaction term to zero. The diffusive flux is defined as

$$\boldsymbol{J}_i = -\left(\rho D_i + \frac{\mu_t}{S_{ct}}\right)\nabla Y_i \quad (6)$$

where D_i is the diffusion coefficient for the ith species in the mixture. S_{ct} is the turbulent Schmidt number defined as

$$S_{ct} = \frac{\mu_t}{\rho D_t} \tag{7}$$

where μ_t is the turbulent viscosity and D_t is the turbulent mass diffusivity.

In the current paper, the scalar transport equation is implemented into *pimpleFoam*, a transient, incompressible OpenFOAM fluid flow solver [7].

2.3. Boussinesq like approximation to account for density differences

An issue with the advection-diffusion specie transport as described by equation (5) is its inability to account for gasses of different densities. In this section we apply a Boussinesq like approximation, which is often used to approximate thermal buoyancy, for mild to minor density variations [6,4].

We continue to assume that density is constant, and hence continue to treat the fluid as an incompressible medium. The effects of density differences between multiple gas sources, only enter into the momentum equation through the body forces $\boldsymbol{F}$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \boldsymbol{u} + \frac{1}{\rho}\boldsymbol{F}. \tag{8}$$

The body force is defined as

$$\boldsymbol{F} = \rho_k \boldsymbol{g}, \tag{9}$$

where $\boldsymbol{g}$ is the gravitational acceleration and ρ_k is the relative density.

For the purposes of the current paper, we distinguish between two gasses only. Therefore given ambient air density of ρ_a and a second gas with density ρ_s with a local mass fraction Y, the relative density is defined as

$$\rho_k = (Y\rho_s + (1 - Y)\rho_a) - \rho_a, \tag{10}$$

where as before, the mass fraction advection-diffusion is described by equation (5).

Given the inclusion of the body force, requires a redefining pressure such that

$$p' = p - \rho_k \boldsymbol{g} h, \tag{11}$$

where, for a fluid at rest, under hydrostatic balance, $p' = 0$.

The Bousinesq approximation has been shown to be accurate as long as the comparative differences in densities are small, typically for cases where

$$\frac{\Delta\rho}{\rho} \ll 1 \tag{12}$$

which is not strictly satisfied for test problem we analyse in Section 3.

The benefit of the current gravity body force approximation is that we can continue to treat the fluid as an incompressible medium and hence can continue to make use of standard, well developed and efficient incompressible solvers. Unfortunately however, the scalar transport equations are no longer decoupled from the momentum equation.

As with the scalar advection-diffusion equation, the Boussinesq like density body force was implemented by modifying the incompressible transient *pimpleFoam* solver.

2.4. rhoReactinBuoyantFoam

rhoReactingBuoyantFoam is an OpenFOAM, density based, compressible, combustion solver which includes chemical reactions with enhanced buoyancy treatment [7]. By turning off chemical reactions, the solver has been shown to be capable of accurately approximating gas dispersion [11,12,13].

By comparison to the two previous incompressible solvers, rhoReactingBuoyantFoam is comparatively complex. *rhoReactingBuoyantFoam* includes compressible continuity and momentum equations, a scalar advection-diffusion transport equation with chemical reactions, an energy equation, a state equation and a pressure-temperature thermophysical model.

While the exact forms of the equations may differ slightly, the general set of equations are as follows. As before the conservation equation is

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0, \tag{13}$$

where the momentum equation for a non-constant density is given by

$$\frac{\partial}{\partial t}(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{g} + \boldsymbol{S} \tag{14}$$

and once again as before the scalar advection-diffusion transport equation

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \boldsymbol{u} Y_i) = \nabla \cdot \boldsymbol{J}_i + S_i + R_i. \tag{15}$$

The energy equation can be defined by

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \boldsymbol{u}) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} K) - \frac{\partial p}{\partial t} = \nabla \cdot \boldsymbol{q} + \nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{u}) + \rho r + \rho \boldsymbol{g} \cdot \boldsymbol{u} \tag{16}$$

where h is the system's enthalpy (the sum of the systems internal energy and dynamic pressure). $\nabla \cdot \boldsymbol{q}$ is the heat flux, where ρr is the heat source for any specific heat source r. K is the specific kinetic energy, defined as $|\boldsymbol{u}|^2/2$, and $\boldsymbol{\tau}$ is the viscous stress tensor and $\boldsymbol{\sigma} = \boldsymbol{\tau} - p\boldsymbol{I}$. For weakly compressible formulation and assuming a perfect gas formulation, density can be related to temperature via

$$\rho = \frac{PM}{RT} \tag{17}$$

where M is the combined fluid mixtures molar weight and R is the universal gas constant. In addition, we have chosen a Sutherland transport model, which defines the dynamic viscosity as

$$\mu = \frac{A_s \sqrt{T}}{1 + T_s/T} \tag{18}$$

where A_s and T_s are constants, set to default values used in OpenFOAM of 1.67212×10^{-6} and 170.672 respectively. While not strictly needed for non-reacting, dense gas dispersion, the *rhoReactingBuoyantFoam* furthermore requires a mixture model (set here to *reactingMixture* model) and a thermo model (set in this case to a *Janaf thermo* model) [7].

Other than deactivating chemistry, no changes were made to the standard OpenFOAM solver.

2.5. Turbulence Model

Turbulence closure models have been shown to be important to accurately model gas dispersion. Based on the numerical experiments presented in [14,15], we have selected the realizable $k - \epsilon$ Reynolds averaged turbulence model. The realizable $k - \epsilon$ has proven to be comparatively accurate when used to model the Thorney Island test case analysed in Section 3.

3. Test Case: Thorney Island Experiment

In this section, we compare the different dispersion models on a simulation of Trial 26 of the Thorney Island field experiments [16]. The Thorney Island experiments were a set of experiments designed to study the dispersion of dense gasses in the presence of obstacles. In Trial 26 of the experiments, a mixture of Freon and Nitrogen was released in the presence of a cubic obstacle. The mixture was composed of 31.6% Freon and 68.4% N_2, resulting in a relative density of 2.0, contained within a 13m tall cylinder with a 14m diameter. In the experiment the cylinder was constructed from flexible material which was allowed to collapse to instantaneously release the dense Freon gas mixture. A 9m*x*9m*x*9m obstacle is situated 50m downwind from the cylinder. The test problem, along with the computational grid, is illustratively shown in Figure 1.

To approximate the experimental conditions, we apply the same boundary conditions as was used in [3, 14, 15]. The inlet boundary condition is approximated using a power law correlation to account for frictional effects, described by

$$u_{\text{in}} = u_0 \left(\frac{z}{z_0}\right)^{\lambda}, \tag{19}$$

where the reference velocity $u_0 = 1.9\,\text{m/s}$ and the reference height $z_0 = 10\text{m}$. λ is a dimensionless parameter which depends on the atmospheric stability, and is set to $\lambda = 0.07$, which corresponds to a 'B' atmospheric stability class under the assumption of moderately unstable atmospheric conditions [17]. The floor is defined as a non-slip boundary condition, where all other boundary conditions are set to be equivalent to open atmospheric boundary conditions. The total computational domain used in this analysis is 300m in length, 260m in width and 80m in height, where the domain is discretised using approximately 1.9million cells.

In the experiment, there were two concentration sensors placed at an elevation of 6.4m on windward face of the obstacle and at a height of 0.4m on the leeward face. The simulation results are shown in Figure 2 along with a comparison of the digitised results of the experimental data and the simulation results presented by Liu *et al.* [3].

The results from the fully compressible, chemistry and combustion solver *rhoReactingBuoyantFoam* compare well to both the results presented in Liu *et al.* and the experimental data. By contrast, both the passive scalar transport and gravity body force approximation was capable of capturing the initial spike on the windward side, but failed to accurately reproduce the leeward data. The inclusion of the relative density body force term does yield an improved approximation when compared to the purely passive scalar transport. Representations of the Freon gas dispersion for the three CFD simulations are shown in Figure 3, shown at intervals of 3, 10 and 20 seconds respectively.

By comparison, all three CFD models outperformed the Guassian dispersion model which predicted a gas leak volume percentage concentration of 0.273% and 0.24% at the windward and leeward sides respectively; this in comparison to expected concentration levels of approximately 6%-10% on the forward face and approximately 2%-2.5% on the leeward face based on the experimental and numerical CFD simulation results. The Gaussian dispersion results were obtained by assuming a constant gas leak, under the assumption of 'B' class atmospheric stability at a dispersion height of 4.5m.

4. Conclusion

In this paper we introduced four different gas dispersion models, namely the popular Gaussian dispersion model, an incompressible scalar specie transport model, an incompressible model with an approximation of the gravitational body force, and finally, a fully compressible, density based CFD solver.

We demonstrated that the OpenFOAM solver, *rhoReactingBuoyantFoam*, despite primarily having been designed to model combustion with thermal buoyancy effects, can be used to accurately predict dense gas dispersion. The results obtained by using the compressible chemistry solver compared well to those presented in [3] as well as the experimental data from Trial 26 of the Thorney Island experiments.

By comparison, the two incompressible, scalar specie transport, CFD solvers were largely incapable of accurately approximating the gas dispersion. The additional gravitational body force, which was implemented in the spirit of a Boussinesq like approximation, was shown to offer only a slight improvement over the purely incompressible approximation, and not strictly valid for the large density difference. It is therefore questionable whether this minor improvement warrants the additional cost. The purely incompressible scalar transport approximation allows for the fluid flow and gas dispersion equations to be separated, which in turn allows for multiple gas dispersion scenarios to be

analysed using a single pre-computed flow solution. The incompressible buoyant approximation negates this benefit, and is therefore only slightly more efficient than the fully compressible *rhoReactingBuoyantFoam* solver.

Our results further confirmed that the current test case falls outside the range of validity of the Gaussian dispersion model, which should be used with caution for near field dispersion or in the presence of obstacles.

Overall, our findings suggest that a purely incompressible assumption can be used to gain order of magnitude estimates, and may prove useful for scenario planning when a multitude of different gas leak scenarios is needed. However, should accurate approximations be required for gas dispersion with large density difference, our advice would be to make use of fully compressible gas dispersion solver, for which OpenFOAM has been shown to be a suitable candidate.

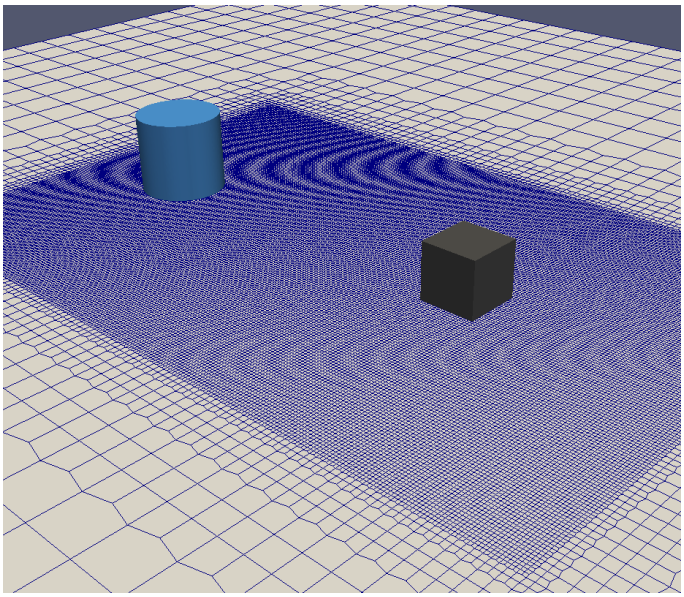

Fig. 1. Schematic of the Thorney Island test Trial 26 problem along with an illustration of the computational grid.

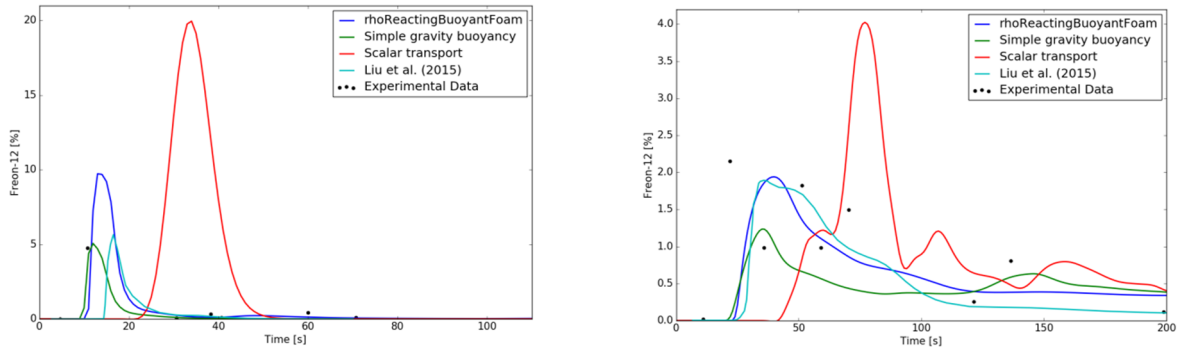

Fig. 2. Comparison of the simulation results for the Thorney Island experiment test Trial 26 showing concentration results at (a) 6.4m elevation on the windward face and (b) 0.4m on the rear face. All three CFD simulation results are compared to the experimental data as well as those reproduced from Liu *et al.* [3].

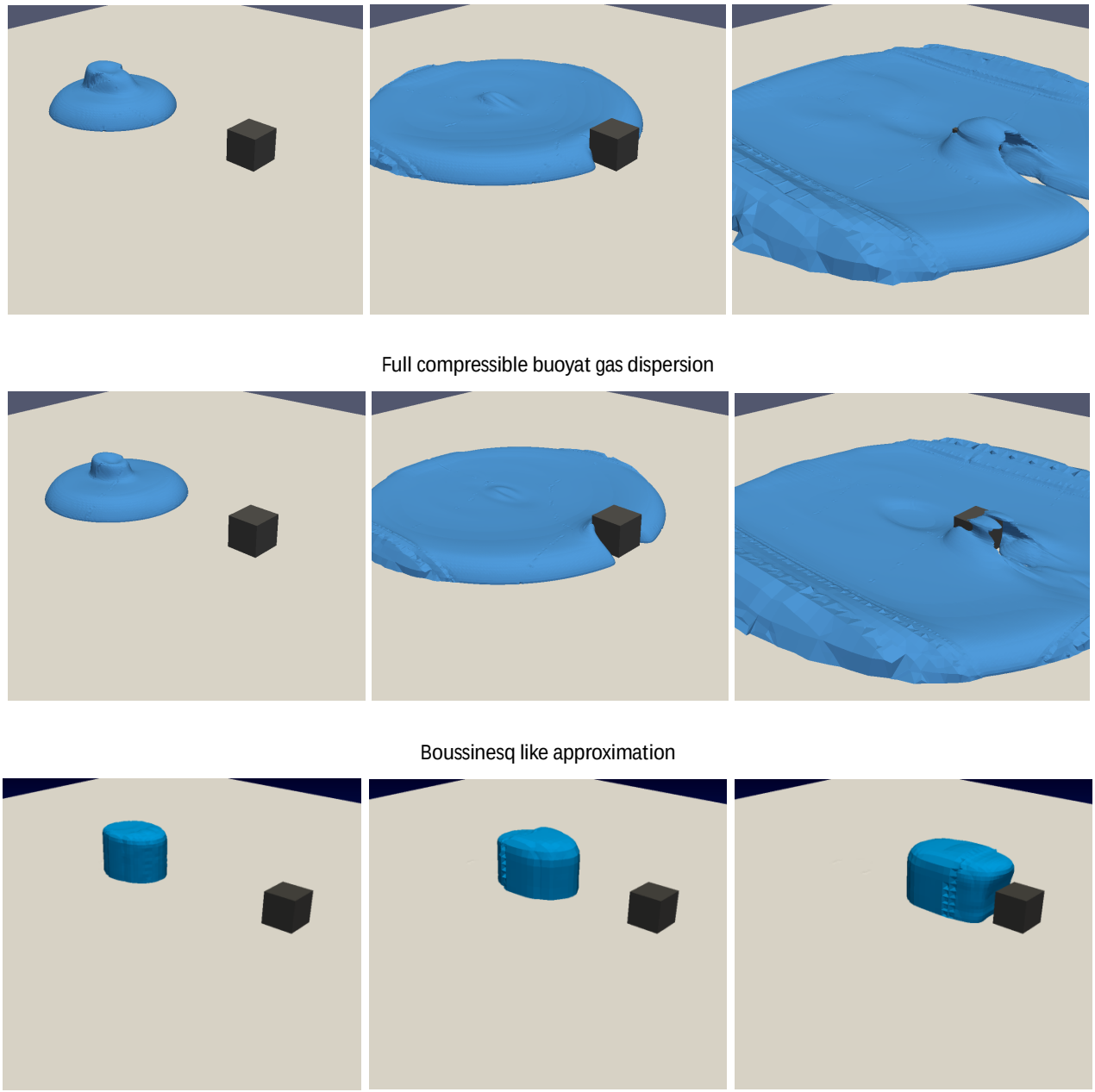

Fig. 3: Gas dispersion comparison using the three CFD models.

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