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A SHALLOW WATER MODEL FOR DENSE GAS SIMULATION IN URBAN AREAS

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1. INTRODUCTION

Large quantities of toxic chemicals are stored at industrial facilities and transported around the country via train and truck. In the event of an accidental release, many of these chemicals are released as heavier-than-air gases that stay low to the ground as they are transported by the wind. Breathing height concentrations can remain high due to reduced vertical mixing and hazard zone coverage area can be larger due to near-source gravitational slumping. A number of fast-response dense gas dispersion models have been developed and are routinely used to deal with heavier-than-air releases over unobstructed terrain. If a release were to occur in a built-up environment, however, the effects of buildings and other obstacles will significantly alter the initial spreading, the transport direction, and the amount of mixing of the dense gas cloud. We have developed a new fast-running dense gas dispersion model that is intended for handling releases in cities and at large industrial facilities. In this paper we describe the scheme employed and how the model has been integrated into the Quick Urban & Industrial Complex (QUIC) dispersion modeling system.

2. BACKGROUND

In the last 30 years, both theoretical and experimental investigations have supported the study of dense gas transport and dispersion behavior, *e.g.*, Thorney Island (McQuaid and Roebuck, 1984), FLADIS (Nielsen and Ott, 1996), Coyote (Goldwire *et al.*, 1983a and b), Burro (Koopman *et al.*, 1981; Koopman *et al.*, 1982), and Goldfish (Blewitt *et al.*, 1987). Dense gas models that have been developed can be divided into three groups:

- integral models that describe the bulk properties of the cloud;
- models based on the shallow water equations (SWE) that consider depth-averaged quantities; and
- computational fluid dynamics (CFD) models that solve the Navier-Stokes equations and a scalar concentration equation.

The final use and the types of problems a model is applied to (*e.g.*, permitting, emergency preparedness, emergency response, accident investigation, operator training) determine the choice of one of the aforementioned groups. For instance, CFD models have been used for recreating accidents to better understand the event (Dharmavaram *et al.*, 2005; Hanna *et al.*, 2009). However, CFD models are not appropriate for emergency response, where a prompt estimation of the accident consequences is necessary. Nonetheless, it is worth noting that the future improvement of both computer hardware and software will probably modify the suitability of different models.

A number of fast-running integral dense gas models and modeling systems were developed in the 70's, 80's, and 90's that have successfully dealt with the phenomena characterizing dense gas dispersion over unobstructed terrain, *e.g.*, SLAB (Ermak, 1990), HEGADAS (Witlox, 1994), DEGADIS (Havens and Spicer, 1985), SCIPUFF (Sykes *et al.*, 1998), ALOHA (Reynolds, 1992). A few attempts have been made to account for the effects of an isolated building or fence in integral dense gas dispersion models (e.g., Rottman *et al.*, 1985), however, they have not been widely utilized nor have they been developed for more complex building arrangements.

We chose to focus on the SWE in order to develop a relatively fast-running dense gas model that can handle complex environments, *e.g.*, chemical facilities, urban areas, and natural topographical features. The SWE are a system of partial differential equations describing the cloud height and the spreading velocities in the horizontal directions. The cloud density is inferred from the cloud height and the entrained volume of air. This paper discusses the modifications made to the traditional SWE in order to approximate dense gas behavior and to account for the effect of buildings and topography. In addition, our preliminary step of merging the scheme with the QUIC random-walk dispersion model is described.

3. DENSE GAS MODEL DESCRIPTION

a) Shallow Water Equations

The shallow water equations (SWE) describe the flow dynamics of an incompressible fluid of constant density in terms of cloud height (h) and horizontal velocities (u, v):

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$$\begin{cases} \dfrac{\partial h}{\partial t} + \dfrac{\partial hu}{\partial x} + \dfrac{\partial hv}{\partial y} = 0 \\ \dfrac{\partial u}{\partial t} + \dfrac{\partial u^2}{\partial x} + \dfrac{\partial uv}{\partial y} + g'\left(\dfrac{\partial e}{\partial x} + \dfrac{\partial h}{\partial x}\right) + S_{fx} = 0 \\ \dfrac{\partial hv}{\partial t} + \dfrac{\partial uv}{\partial x} + \dfrac{\partial v^2}{\partial y} + g'\left(\dfrac{\partial e}{\partial y} + \dfrac{\partial h}{\partial y}\right) + S_{fy} = 0 \end{cases} \qquad (1)$$

where e is topographical elevation, g' is $(\rho-\rho_a)/\rho_a$, ρ is the cloud density, ρ_a is the ambient air density, and S_{fx} and S_{fy} represent the friction factors. The ground slope terms ($\partial e/\partial x$ and $\partial e/\partial y$) account for the effects of drainage resulting from topography. All the dependent variables are depth-averaged, *i.e.*, the model assumes they are constant. The model has been formulated to allow for either an instantaneous, finite duration, or continuous (non-elevated) release of any shape or size.

The PDE system is solved with the finite difference method on a rectangular grid of assigned dimensions. The solution approach is based on discretizing spatially the PDE into a system of ordinary differential equations which are then numerically integrated by means of Euler's forward method. A stable solution is obtained by forcing the time step to satisfy the Courant–Friedrichs–Lewy condition (Strikwerda, 1989): $dt = 0.3 \times \min(dx/u,\ dy/v)$. We use the upwind scheme to discretize the PDE in the spatial derivatives.

b) Modifications for Dense Gases

The SWE applied to dense gases must be modified in order to account for density variation with time due to dilution with fresh air. The most straightforward method is to add another partial differential equation for the density dynamics, *e.g.*, Ott and Nielsen (1996), Venetsanos *et al.* (2003), and Folch *et al.* (2007). However, due to our need for a faster model, we chose an approach where the dilution step is done separately.

Both Fay and Ranck (1983) and Eidsvik (1980) stated that the horizontal spreading of a dense cloud is almost independent from the air entrainment process for isothermal releases. Hanna and Drivas (1987) used this hypothesis to develop an integral (box) model. Consequently, for isothermal releases, it is possible to solve the SWE derived for fluids of constant density and determine the dilution *a posteriori*. After each time step in the solution of the partial differential equations (PDE) describing the cloud height and the horizontal spreading velocities, the cloud density is inferred from the cloud height and the air entrainment velocity (w_e). The entrainment velocity is parameterized based on Eidsvik (1980), but also accounts for the difference between the outflow velocity of the slumping cloud (u_g) and the mean velocity of the surrounding air (u_a):

$$w_e = \frac{a_1 u_* + a_2\left|u_a - u_g\right|}{1 + a_3 Ri} \qquad (2)$$

where u_* is the friction velocity, Ri is the Richardson number, and the constants are specified according to Hankin and Britter (1999): a_1 = 0.4, a_2 = 1, and a_3 = 0.125.

c) Accounting for Buildings

The ground slope terms in eqn. (1) are not used to evaluate the flow around buildings and other obstacles. Doing so can result in unrealistic cloud behavior. Rather, we developed rules that don't allow the dense gas cloud to penetrate the obstacles, but do allow the cloud to flow over the top of an obstacle if it is higher than the obstacle itself.

Although not fully implemented at the time of writing this paper, the code is being developed to utilize the wind field computed by the QUIC wind solver (*e.g.*, Pardyjak and Brown, 2001 and 2003). As described in Singh *et al.* (2008) and Gowardhan *et al.* (2008), the QUIC wind solver is a fast-running empirical-diagnostic code used to compute 3D wind fields around large clusters of buildings. The complex wind fields produced by QUIC are used to transport the dense gas cloud through the obstacles, although the QUIC-computed wind field must be averaged through the depth of the dense gas cloud owing to the constraints of the SWE. In addition, the QUIC wind field is used to define the reference velocity for the entrainment term (eqn. 2), so that the dilution can differ in each portion of the dense gas cloud.

d) Accounting for Transition to Neutral Density

Shallow water dense gas models are only valid during the early stages of dispersion before dilution has rendered the cloud nearly neutral. Since the cloud is often still dangerous long after it has become a passive gas, the shallow water model must transition or be linked to a passive gas dispersion model. As part of the QUIC modeling system (Williams *et al.*, 2004), Williams *et al.* (2005) developed dense gas algorithms for instantaneous and continuous releases in the vicinity of buildings using integral methods combined with a random-walk transport and dispersion model. In the current modeling system, we replace the simpler integral slab model with the SWE. In this approach, the random-walk marker particles are uniformly distributed inside the initial source volume and then given the dense gas slump velocities as computed by the SWE and the winds produced by the building-aware QUIC wind model. The turbulence within the dense gas cloud is reduced according to a term inversely proportional to one plus the cloud Richardson number. Marker particles can escape the dense gas cloud via the turbulent velocities or the vortices created by the buildings (*e.g.*, an updraft on the back side of the building). Thus the model allows for determination of material emitted from the dense gas cloud. Once outside the dense cloud, the marker particles are treated as passive neutral tracers. When the cloud is diluted enough to approach neutral conditions, *i.e.*, the Richardson number goes to zero, a smooth transition is obtained since the same random-walk model continues to be used for the transport and dispersion but without the SWE input.

4. MODEL RESULTS

a) Verification

The verification step is the process of checking that a numerical procedure solves the equations correctly. The verification process compares the model results with those of a standard model that was validated for some specific configurations of the system. To verify the dense gas dispersion model discussed in the previous sections, we compared its output with the box model of Hanna and Drivas (1987) for instantaneous releases. The case study comprises a heavier-than-air cylinder release with 9.3 m radius, 14 m height and 3 kg/m^3 initial density. The wind speed at 10 m is 2 m/s.

Figure 1 shows the comparison between the cloud radius, height, and density evaluated with our SWE model and the box model of Hanna and Drivas (1987). These figures show the time variation of the cloud radius, height, and density until dilution makes it neutral. The top two panels in Figure 1 show that the SWE modified model reproduces the expected behaviors. The radius increases in time due to the negative buoyancy of the cloud that makes it slump on the ground. Initially, the height decreases due to the slumping, and then it slightly increases because of the dilution with air. The density decreases monotonically due to the air entrainment and the consequent increase of the cloud volume.

b) Urban Application – No Ambient Winds

As a first test, we have applied the shallow water dense gas model to a non-ideal array of buildings with no cross flow. Figure 2 shows the slumping and subsequent dispersion of the dense gas around the low-rise buildings. As can be seen, the cloud shape is initially axisymmetric, approximating a cylinder. The building obstacles stop the cloud spreading and force it to disperse laterally. As the cloud travels down streets it is apparent that there is some speed up of portions of the cloud front as it gets channeled into narrow streets. The SWE dense gas model is shown to produce qualitatively realistic results, although an extensive and detailed validation is warranted.

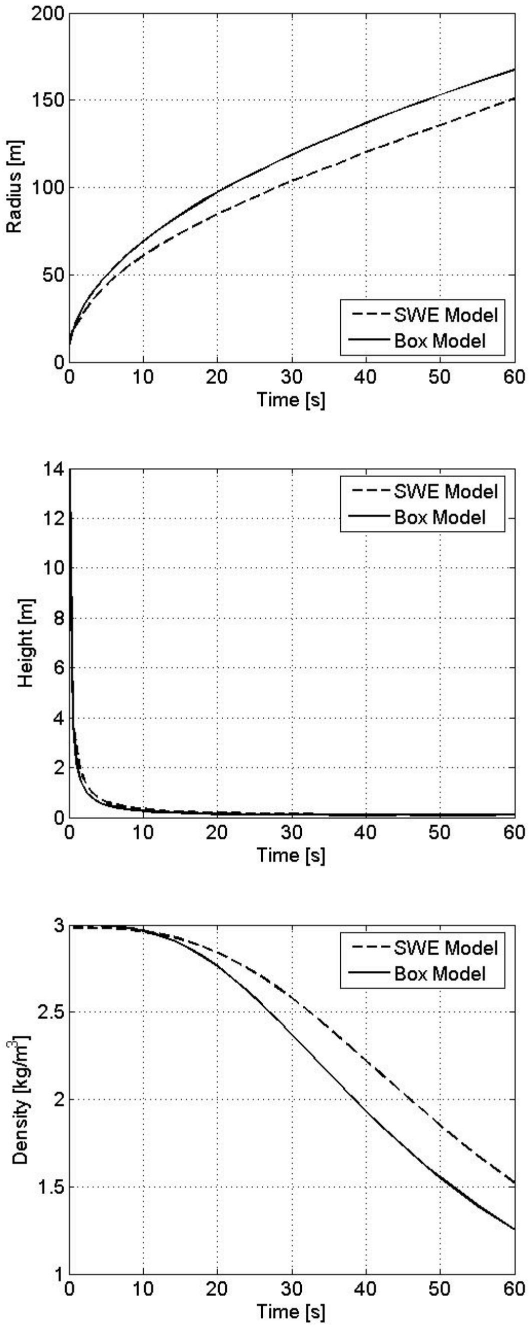

Figure 1: Variation of the radius (top), the height (middle), and the density (bottom) of the dense gas cloud with time computed by the shallow water model (dashed line) and a box model (solid line).

5. CONCLUSION

The shallow water equations represent a suitable methodology to simulate dense gas dispersion in both industrial and urban areas because they account for both the topography and the presence of obstacles. The entrainment can be parameterized using approaches such as that proposed by Eidsvik (1980). For flat terrain with no cross flow, we demonstrated that the shallow water dense gas model reproduced the expected trends of cloud height, radius, and density and matched the standard box model of Hanna and Drivas (1987) fairly well.

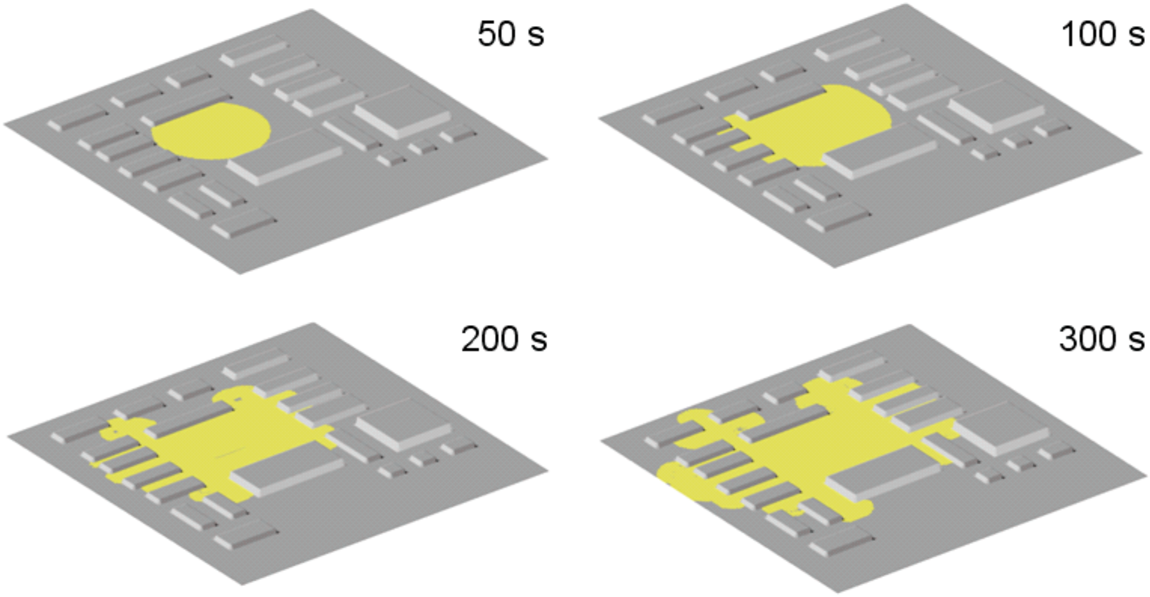

Figure 2. The shallow water dense gas model applied to a built environment under calm winds.

We have integrated the shallow water solver into the QUIC dispersion modeling system. This has several advantages. The QUIC wind solver will provide a spatially-variable reference velocity to quantify the air entrainment in and around buildings. The QUIC random-walk dispersion model is used with the cloud produced by the SWE in order to ensure a smooth transition between the dense gas phase and the neutral gas phase, as well as to better model the exfiltration of material out of the dense gas cloud. The horizontal velocities evaluated by solving the SWE are used to drive the random-walk marker particles in order to capture the slumping effect.

We have demonstrated that the model appears to give qualitatively plausible results for a non-ideal building layout. Future work will be devoted to completing the integration within the QUIC modeling system, the addition of droplet evaporation thermo-dynamics, the verification of continuous releases and the validation of the model with experimental and wind-tunnel data.

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