Journal of Hazardous Materials 280 (2014) 436–449

Contents lists available at ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Modeling blast waves, gas and particles dispersion in urban and hilly ground areas

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HIGHLIGHTS

- An hydrodynamic model involving large cells containing obstacles is built.
- A new model for particles flow, including turbulent effects is developed.
- A 3D code predicting dispersion phenomena in heterogeneous media is presented.
- Numerical elevation data are used to rebuild the topography of the considered media.

ARTICLE INFO

Article history:
Received 2 May 2014
Received in revised form 31 July 2014
Accepted 4 August 2014
Available online 17 August 2014

Keywords:
Fluid dispersion
Two-phase flow
Heterogeneous media
Compressible flow

ABSTRACT

The numerical simulation of shock and blast waves as well as particles dispersion in highly heterogeneous media such as cities, urban places, industrial plants and part of countries is addressed. Examples of phenomena under study are chemical gas products dispersion from damaged vessels, gas dispersion in urban places under explosion conditions, shock wave propagation in urban environment. A three-dimensional simulation multiphase flow code (HI2LO) is developed in this aim. To simplify the consideration of complex geometries, a heterogeneous discrete formulation is developed. When dealing with large scale domains, such as countries, the topography is considered with the help of elevation data. Meteorological conditions are also considered, in particular regarding complex temperature and wind profiles. Heat and mass transfers on sub-scale objects, such as buildings, trees and other obstacles are considered as well. Particles motion is addressed through a new turbulence model involving a single parameter to describe accurately plumes. Validations against experiments in basic situations are presented as well as examples of industrial and environmental computations.

1. Introduction and background

In many natural and industrial situations, it is important to predict the dynamics of blast wave, gas and particles dispersion resulting of an explosion. At least, two types of difficulties appear when dealing with such numerical simulations. First, the topology of the medium under interest may be very complex regarding the presence of obstacles or objects of different types. Second, large disparities in both space and time scales often require attention. This is the case when dealing with the dispersion of gases from explosions in strongly heterogeneous media such as urban places, cities and hilly grounds.

Various existing computational codes are available in this area: FLACS, developed for many years and widely documented ([1–5] and [51]), CFD-URBAN [6] or FEFLO [7–9]. These codes are used to predict gas clouds dispersion in complex geometries such as cities and industrial sites and allow the study of risk explosion. The approach promoted in the present work is similar to the one adopted in the FLACS code regarding topology and geometrical considerations. FLACS takes into account the geometry details with the help of an internal porosity allowing the presence of obstacles within the control volume. The porosity approach is used since many years to model forest or obstacles, readers can refer [49,53,54] or [58]. FEFLO is an unstructured finite-element finite volume code able to describe complex geometries with the help of sophisticated

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http://dx.doi.org/10.1016/j.jhazmat.2014.08.011
0304-3894/

mesh generator. FEFLO-URBAN allows the presence of trees with a forest model based on a porosity approach [53]. CFD-URBAN is able to model fluid flows and concentration dissemination in domains such as cities, but in the absence of shocks or blast effects.

Alternatively, many hydrocodes are available to model blast effects, such as AUTODYN [10], Air-3D [11] or SHAMRC [12]. These codes are aimed to study unsteady phenomena such as shock waves propagation in the presence of buildings, in the context of moderate geometrical complexity. Thus, there are mainly two existing strategies to consider both blast effects and gas dispersion in complex media:

- Flow solvers based on unstructured grids, such as FEFLO.
- Cartesian grid solvers with an internal porosity, such as FLACS.

The present work belongs to the second class, with a heterogeneous media model built on the basis of rigorous mathematical basis. A discrete model [13] is developed to deal with gas dynamics in highly heterogeneous media. In addition, particles cloud dispersion effects are considered through a pressureless gas dynamics model including turbulent effects fully coupled with the gas dynamics equations. In the present heterogeneous media, obstacles of very different sizes may be present. Large Eddy simulation (LES) is no longer appropriate to solve the gas dynamics equations over such complex topographies, as the time to generate the mesh is prohibitive, as well as the computational time on long time scale events. Thus a homogenized model with cells of large dimensions containing obstacles is more appropriate [13]. This type of model belongs to the class of averaged multiphase flow models as described in [14,15] but with a single phase, the other phase corresponding to motionless obstacles. The model considers the volume occupied by the solid obstacles as well as their effects on the macroscopic flow dynamics. In this aim, the local pressure forces are determined by considering internal boundaries and specific Riemann solvers, or specific boundary solvers. In that sense, the method presented in this paper is quite close to embedded boundary methods (or cut-cells) approaches [16,17] when dealing with the geometry description. It differs when very small obstacles are present, such as trees for which the exchange surface is not those of the cut-cell.

We summarize in the present paper the discrete model of [13] and extend it to mass concentration determination as well as particle dynamics equations. In this aim, the high order ADER scheme [18,19] is used to reduce the numerical diffusion and compute accurately gas concentration fields. Mass diffusion and heat exchanges are introduced both at macroscopic and sub-scale levels. Last, examples of simulations on urban and on very large scales are presented to show capabilities of the three-dimensional simulation code.

2. Heterogeneous model building

To build the discrete model of heterogeneous media, a two phase control volume containing a gas and a motionless solid is considered. The equations for the dispersed phase (solid particles) will be considered later. The gas phase is governed by the multicomponent Euler equations, dissipative effects being considered later as well.

2.1. Gas dynamics equations

The equations to consider in the gas phase are the multicomponent gas dynamics equations:

$$\frac{\partial \vec{U}}{\partial t} + \nabla \cdot \vec{F} = 0 \qquad (1)$$

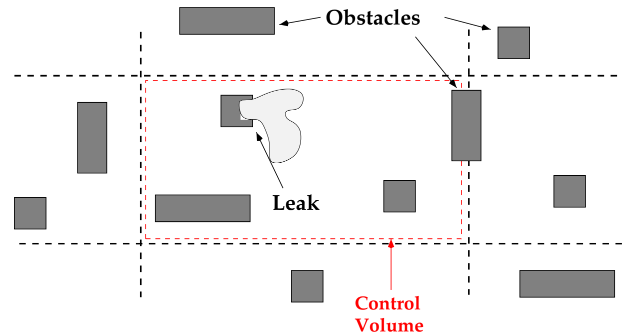

Fig. 1. Representation of the heterogeneous control volume. Internal obstacles can potentially burst, inducing gases leakages within the cell.

where $\boldsymbol{U}$ represents the conservative variables vector and $\boldsymbol{F}$ the fluxes vector:

$$\vec{U} = (\rho Y_K, \rho, \rho\vec{u}, \rho E)^T,$$

$$\vec{F} = \left(\rho Y_K \vec{u}, \rho\vec{u}, \rho\vec{u} \otimes \vec{u} + P\underline{\underline{I}}, (\rho E + P)\vec{u}\right)^T$$

ρ, $\vec{u}$ and P represent respectively the mixture density, the velocity vector and the pressure. Y_k is the mass fraction of the chemical species k and E is the total energy, defined by:

$$E = \frac{\left\|\vec{u}\right\|^2}{2} + e(T, Y_k)$$

$$e(T, Y_k) = \sum_{k=1}^{N} Y_k e_k(T)$$

$$e_k(T) = \int_{298}^{T} c_v dT + e_k^{298}$$

The thermodynamic closure of System (1) is given by the ideal gas equation of state for the mixture:

$$\frac{1}{\hat{W}} = \sum_{k=1}^{N} \frac{Y_k}{W_k}$$

With $P = \rho RT$ and R, the mixture gas constant: $R = \hat{R}/\hat{W}$ with $\hat{W}$ the molar mass of the mixture.

2.2. Integration on heterogeneous control volume

System (1) is integrated on a heterogeneous control volume containing both fluid and solid (as shown in Fig. 1) and over a time step. Space and time integration provide the discrete heterogeneous model. The procedure starts with,

$$\int_{t^n}^{t^{n+1}} \int_{V_i} \left\{ \frac{\partial U}{\partial t} + \nabla \cdot F \right\} dVdt = 0$$

where V_i corresponds to the fluid volume within the cell, which is not necessarily equal to the cell volume, because of the possible presence of internal solid obstacles. The mass conservation equation is integrated hereafter, as a calculation example. The following integrals have to be computed.

$$\int_{t^n}^{t^{n+1}} \int_{V_i} \frac{\partial \rho}{\partial t} dVdt + \int_{t^n}^{t^{n+1}} \int_{V_i} \rho(\vec{u} \cdot \vec{n}) dVdt = 0 \qquad (2)$$