Sudden release of hazardous substances - CFD modelling of dispersion process

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Highlights

- A dispersion model of pollutants was developed using CFD methods.
- The effects of atmospheric conditions on the dispersion of pollutants were simulated.
- The influence of thermal ignition on ethylene combustion was determined.

1. Introduction

The mathematical modeling of sudden release of dangerous substances into the atmosphere is presented as a basic method for creating emergency scenarios. For this purpose, two types of mathematical models are used: the analytical and numerical ones, respectively. For analytical considerations, mathematical models based on the Gaussian plume model are employed. While for numerical modeling, a computational fluid dynamic - CFD, which enables a mathematical description of the turbulent diffusion phenomena, is used. With CFD models, after solving the appropriate set of momentum, mass and energy equations, a lot of information on the modeled system can be obtained in a discrete manner. In this paper, we present a method to formulate the standard inlet conditions for description of turbulent flow, following the proposal given by Richards and Hoxey (1993). However, these conditions require a determination of either the hydraulic diameter of region in which the dispersion process occurs or the thickness of laminar boundary layer in this system. The thickness of the laminar boundary layer at the inlet to the region is zero, this generates a big problem in description of process with use of CFD methods. An iteration method to determine the standard inlet conditions for turbulent flow is also presented. The turbulent viscosity and turbulent Schmidt number as well closure methods for momentum transfer have been used for this purpose. As a result, an influence of the chosen turbulence model on the spread of pollutants is checked. Performed numerical simulations are verified with use of experimental research obtained by Tominaga and Stathopoulos (2012).

2. Methods

In mathematical modeling of the pollutants transport with use of CFD methods, the closure hypothesis to close of the Navier-Stokes is applied. Based on these models, the turbulent Schmidt number can be estimated within the area under consideration. The mass balance of i-th component dispersed within the ambient can be written as follows:

$$\frac{\partial \overline{C_i}}{\partial t} + \bar{u}_i \frac{\partial \overline{C_i}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_T}{Sc_T} \cdot \frac{\partial \overline{C_i}}{\partial x_i} + D_{ij} \frac{\partial \overline{C_i}}{\partial x_i} \right) + \nu_i R$$

The analysis of the subject literature dealing with this issue shows that this way of describing turbulent diffusion is quite often used. Table 1 summarizes data given in some representative papers. In articles where CFD models have been verified with use of the experimental data, the values of turbulent Schmidt number range with <0.2-2>. For the simulations performed in this work, the value of $Sc_T = 0.7$ was chosen as the most commonly used to describe the dispersion of pollutants in the gas phase.

Table 1. Mathematical modeling of turbulent diffusion - literature review

Author	Model of turbulence	Sc_T
Gousseau, 2011	k-eps, LES	*0.3;0.5;0.7*
Karim, 2011	k-eps	*1.3*
Steffnes, 2013	k-eps, RSM, LES	*not reported*
Tominaga, 2012	k-eps RNG,LES	*0.2-2 (0.7)*

3. Results and discussion

Simulations of pollutant dispersion have been performed for systems of different concentrations of pollutant in the source and ambient conditions. Figure 1 shows the distribution of concentration of released ethylene in a hypothetical street. Also, the case with ignition was investigated. An influence of ignition energy on the process was also taken into account.

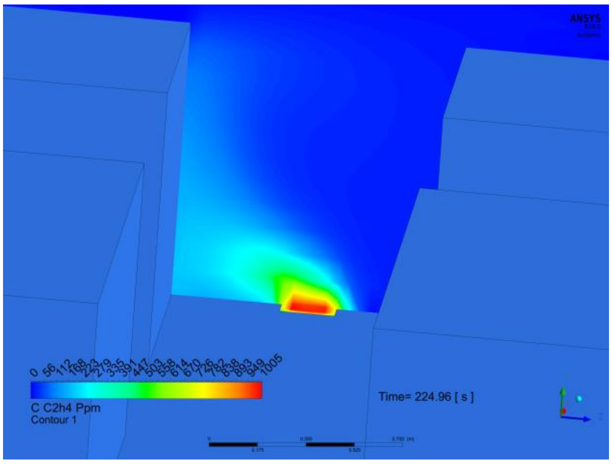

Figure 1. Distribution of ethylene concentration (C [ppm]) in time equal t = 224.96 [s].

4. Conclusions

Mathematical modeling of turbulent diffusion allows to describe the process of diffusion of dangerous substances in the ambient. Such an approach allows us to balance the mass of the component but also the momentum and energy. The disadvantage of these methods is the high demand for computational power of computers to carry out the simulations.

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