

# Modelling of dense and neutral gas dispersions - LPg, methane and methanol

📅 25.07.2016

## Modelování disperze těžkého a neutrálního plynu - LPG, metan a metanol

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plyny

metan

metanol

disperze

modelování

### Abstract

The use of liquefied natural gas, methanol, methane and hydrogen as fuels brings up issues regarding safety and acceptable risk. The potential hazards associated with an accidental release and dispersion should be evaluated. The article reports the results of different methods of modelling releases and dispersion of dangerous gases and vapors in cases of major accidents in industrial or urban zones. To describe these methods we introduce how parameters (such as amount of release gas, atmospheric conditions, buildings, tanks cracks, diameter etc.) at an industrial or urban site affect dispersion and show how these parameters can be parametrized in effects models. Effect evaluation is an important part for mitigation factors, such as water sprays, foam systems, and sheltering or evacuation, which tend to reduce the magnitude of potential effects in real incidents. The goal of this article is to present the results of modelling using these standard methods in the area of modelling of releases and dispersions of dangerous chemical substances in urban zones in cases of major accident.

**Keywords:** Modelling of release and dispersion, Effects 9.0.8, Aloha 5.4.6, CPQRA, gas/vapor

### Abstrakt

Používání zkapalněného zemního plynu, metanolu, metanu a vodíku jako paliva vyvolává otázky týkající se bezpečnosti a přijatelnosti rizika. Tato potenciální rizika spojená s náhodným únikem a rozptylem by měla být hodnocena. Článek uvádí výsledky různých metod modelování úniků a rozptylů nebezpečných plynů a par v případech závažných havárií v průmyslu nebo v městských zónách. K popisu těchto metod jsme představili, jak parametry (například množství uniklého plynu, atmosférické podmínky, stavby, průměr trhliny v nádrži) v oblasti průmyslového nebo městského typu ovlivňují rozptyl a ukázali, jak mohou být tyto parametry parametrizovány v modelech efektů. Vyhodnocení efektů je

důležité pro opatření ke zmírnění následků, jako jsou vodní stěny, pěnové systémy, ukrytí nebo evakuace, které mají tendenci snižovat závažnost potenciálních efektů. Cílem tohoto článku je prezentovat výsledky modelování pomocí standardních metod v oblasti modelování úniků a disperzí nebezpečných chemických látek v městských zónách v případě závažné havárie.

**Klíčová slova:** Modelování úniku a rozptylu, Effects 9.0.8, Aloha 5.4.6, CPQRA, pára/plyn

## Introduction

The three major physical effects occurring during accidents - fire, explosion and toxic release - usually involved emission of material from containment followed by vaporization and dispersion of the material. The treatment given here is relevant to all three major physical effects occurring during accidents; in particular, the development of the emission and dispersion phases is relevant to such situation as: Escape of flammable material, mixing of the material with air, formation of a flammable cloud, drifting of the cloud and finding of a source of ignition, leading to (a) a fire and/or (b) a vapor cloud explosion, affecting the site and possibly populated areas [1].

When assessing the (lack of) safety of accidents with hazardous substances, calculation (or prediction) of the consequences of an accidental release of the substance plays a crucial role. The accident scenario (the course of an accident) passes through a number of phases of behavior of the released substance. These phases are dependent on: the nature of the substance (e.g. is it a gas, a liquid or a solid), the risk potential of the substance (is it flammable/explosive, or does the danger lie in the toxicity), the circumstances under which the substance is stored and is released (e.g. at high pressure or temperature), the ambient conditions (external temperature, wind speed, complex buildings or open air) [2].

Accidents begin with an incident, which usually results in the loss of containment of material from the process. The material has hazardous properties, which might include toxic properties and energy content. Typical incidents might include the rupture or break of a pipeline, a hole in a tank or pipe, runaway reaction, fire external to the vessel, etc. Once the incident is defined, source models are selected to describe how materials are discharged from the process. The source model provides a description of the rate of discharge, the total quantity discharged (or total time of discharge), and the physical state of releasing (discharging) material, that is, solid, liquid, vapor or a combination. A dispersion model is subsequently used to describe how the material is transported downwind and dispersed to some concentration levels. For flammable releases, fire and explosion models convert the source model information on the release into energy hazard potentials such as thermal radiation and explosion overpressures. Effect models convert these incident-specific results into effects on people (injury or death) and structures [3].

## Description of methodical approaches

In the present study, two methodologies developed in [6-7] are applied to the estimation and assessment of risks associated with accidental releases of dangerous flammable substances. In order to manage these risks effectively, they must be estimated. Since risk is a combination of frequency and consequence, consequence (or impact) analysis is a necessary step in the risk management process. This article provides an overview of effect models commonly used for the purpose of hazardous zones modelling.

Two computational approaches have been used: 1) methodology [3] with simplest calculations that require an estimate of the release rate of the gas (or the total quantity released), the atmospheric conditions (wind speed, time of day, cloud cover), surface roughness, temperature, pressure and release diameter; 2) representative software packages ALOHA 5.4.6 [5] and EFFECTS 9.0.8 [4] with complicated models that require additional detail on the geometry, discharge mechanism, and other information on the release.

These computational approaches describe the physical behavior of a substance during and after its release (with specific term "Loss of Containment"). These models calculate the outflow speed, the evaporation of a liquid, the dispersion of vapor in the atmosphere and the resulting concentrations in the external air, the intensity of heat radiation in the case of a fire, the pressure from an explosion, etc. The models for this are described in detail in the so-called "Yellow Book" published by the Committee for the Prevention of Disasters from Hazardous Substances (CPR) [2].

Generally, it might be argued that models currently used in risk assessment and evaluation of the consequences of accidents were developed to fit tasks characterized by boundary conditions and dispersion characteristics that are much more simple compared to those relevant to real urban zones. However, to obtain rough results, these models may be applied; the resulting distances of hazardous zones are then conservative, with many uncertainties in the case of obstacles present (high buildings) [6].

## **Description of accident scenarios**

### **General description**

To calculate the effects of release of a hazardous substance to its environment, a large number of calculation models have been developed which are based on the physical and chemical properties of substances and physical behaviour in general, and on validation experiments for specific, often extreme process conditions. Basically they consist of a pre-described chain of models, linked together into one combined model.

Because a lot of the input parameters of a model can be taken from output of the preceding model, the required input of the combined model is not the same as "all inputs of all models together". Although they are referred as being a model-chain, it is better to think of a combined model as being a tree, because it may consist of several branches.

The scenarios are described as a two-phase flow after the release of liquefied gases, followed by their dispersion. The dispersion of methanol (a flammable liquid) was calculated by pool evaporation after the release. The fatal zones of flammable substances represent 60% of LEL for a potential flash fire or vapour cloud explosion. To approximately match the multiple obstacles in cities, the urban roughness was considered during all Effects and Aloha simulations. Tables summarises all important input data necessary for modelling of releases and dispersion of the selected dangerous substances.

### **Types of accident scenarios considered**

#### **A) Instantaneous scenario**

In case of an instantaneous scenario, the dispersion models will have to run in "instantaneous mode", whereas the source rate from the pool is continues source. For that reason, two dispersion models will need to run. Note that it can occur that the instantaneous flash will be a heavy gas (due to the liquid fraction and temperature), whereas the pool evaporation source may be "neutral". Note the density of the evaporated mass is based on mixing with air of a 0.5 meter window height. After calculation of explosive result, the dispersion results itself are cumulated. For this cumulating of an instantaneous dispersion result, distinction has been made between cumulating of dispersion-explosive models [4].

#### **B) Continuous scenarios**

In case of the continuous scenario, the source rate is of a two phase release determined by: 1) The 2 phase Bottom Discharge (TPDIS) model, followed by spray release, which calculates rainout mass flow rate and a air born flow rate; 2) The pool evaporation, fed by the rain out mass rate will also create a continuous source rate. The dispersion model

has to be fed with important cumulated parameters: combined mass flow rate, representative release duration, and liquid fraction of the mixture. Not that if the input chemical is a pure liquid, the dispersion model will run in "pool evaporation mode" and input will be purely the pool evaporation mass rate (release height 0). If the chemical is a gas, the accumulation routine will skip the pool-input, and the following dispersion model will run in "horizontal jet" mode, with dimensions taken from the jet diameter [4].

### Description of inputs necessary for modelling

Table 1-3 summarises all important input data according to the methodology from [6] necessary for modelling of releases and dispersion of the selected dangerous substances. The most important meteorological conditions influencing the dispersion of dangerous substances are direction and speed of wind, stability class and air temperature. Regarding many possibilities in real situations, the following basic conditions were finally chosen for modelling: The neutral stability of atmosphere [D class; medium wind speed of  $5\text{ms}^{-1}$  (the most frequent conditions during the year→the most probable scenario)]. The very stable stability of atmosphere [F class; low-wind speed of  $1.7\text{ms}^{-1}$  (the worst dispersion conditions, cloud impact of the largest area→the worst case scenario)].

SCENARIO	TYPE OF RELEASE (CONTINUOUS/INSTANTANEOUS)	STABILITY CLASS	WIND SPEED (M/S)	TEMPERATURE (°C)
1	instantaneous	D	5	25
2	instantaneous	D	5	25
3	instantaneous	F	1.7	10
4	instantaneous	F	1.7	10
5	continuous	D	5	25
6	continuous	D	5	25
7	continuous	F	1.7	10
8	continuous	F	1.7	10

Table 1: Summary of atmospheric input data for modelling

SCENARIO	ALOHA		EFFECTS	
	RELEASE RATE (KG/S)	RELEASE DURATION (MIN)	RELEASE RATE (KG/S)	RELEASE DURATION (MIN)
1	151	1	1209	0.12
2	151	1	978	0.16
3	14	12	33	4

4	10	15	27	6
5	363	1	1209	0.28
6	363	1	978	0.38
7	14	28	33	10
8	10	37	27	14

Table 2: Summary of release input data for modelling

<b>GAS</b>	<b>CONCENTRATION [PPM]</b>
LPG	12 600 (60% LEL)
METHANOL	43 080 (60% LEL)
METHANE	30 000 (60% LEL)

Table 3: Summary of endpoint values as input data for modelling

## Results and discussions

Software packages ALOHA and EFFECTS represent well-known pre-accident modelling tools commonly employed in assessment of dangerous substances releases, dispersion, and other effects and consequences. These models are still under construction [6].

The first result of the contribution is to compare the results of previous work that has been made by ALOHA 5.4.1 and EFFECTS 5.5 in comparison with ALOHA 5.4.6 and EFFECTS 9.0.8 for LPG scenario 1.2B. The results of modeling for particular substance LPG, when used with identical data input assumptions, are summarized and compared in Table 4.

<b>SCENARIO</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>
Effects	132 (24)	124 (32)	173 (4)	226 (4)	75 (23)	75 (31)	112 (4)	134 (6)
Aloha	282 (242)	452 (392)	415 (69)	528 (120)	89 (391)	87 (574)	173 (70)	176 (121)
CPQRA	426	600	405	571	168	168	140	140

Table 4: LPG: CPQRA in comparison with ALOHA 5.4.6 and EFFECTS 9.0.8 (results in m)

\* Numbers in the closeres denotes previous study [6]

Tables 5-6 introduce new results obtain for further computation studies.

<b>SCENARIO</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>
Effects	375	496	622	800	69	69	218	226
Aloha	397	589	713	994	119	119	396	396
CPQRA	300	300	102	102	363	250	800	926

Table 5: Methane: CPQRA in comparison with ALOHA 5.4.6 and EFFECTS 9.0.8 (results in m)

<b>SCENARIO</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>
Effects	124	218	276	224	35	35	22	22
Aloha	154	245	234	299	48	48	84	84
CPQRA	435	614	424	598	152	152	146	146

Table 6 Methanol: CPQRA in comparison with ALOHA 5.4.6 and EFFECTS 9.0.8 (results in m)

The following comparisons are discussed before making more general conclusions on the results obtained: a) results based on ALOHA and EFFECTS software calculations; b) distances of hazardous zones fewer than two types of weather conditions (the most frequent versus the worst condition from the point of view of cloud dispersion). Employing models implemented in the EFFECTS software package, the hazardous zones calculated for methane accidents (scenarios 1-8) are depicted in Table 4 (LPG). The results of hazardous zones obtained by ALOHA and EFFECTS software applications are generally similar, at least of the same order that is close to the results obtained by [6]. The greatest difference was for 3-4 and 7-8, where EFFECTS 9.0.8 shows the fatal zones in order of hundreds/tens meters compared with EFFECTS 5.5 in tens/unit of meters only. The greatest difference between ALOHA and EFFECTS for methane was for 1-2 scenarios, where ALOHA shows the fatal zones in order of hundreds different from the results by EFFECTS. There is also great difference between the results taken by EFFECTS and ALOHA in comparison with CPQRA, especially for cases 7-8 (more than 600 m). The difference between ALOHA and EFFECTS for methanol case is negligible. The difference between the CPQRA and the other two programs differs at least in the order of hundreds. With regard to input data identical for both software applications, the calculated release rates differ more than the distances of the hazardous zones (see Table 2, e.g. 1-2 and 5-6).

## Conclusion

A comparison of Effects 9.0.8, Aloha 5.4.6 and CPQRA methods has been carried out as the basis for further study. Model releases and dispersion of dangerous gas (methane) and vapors (methanol, LPG) in cases of major accidents of road and rail transportation in urban zones have been investigated and their possible consequences discussed in our contribution. The program EFFECTS calculates shorter distances of fatal zones in most cases. Thus, the program ALOHA can be described as a more conservative tool from the point of view of risk assessment. Finally, our results can be employed when preparing more sophisticated simulations based on computational fluid dynamics modeling [8-9] and wind tunnel experiments [10], and aimed at investigation of the limitations of standard models on one hand, and their improvement on the other hand.

## Acknowledgement

This work was prepared within the project „Innovation for Efficiency and Environment - Growth“, identification code

LO1403 with the financial support from the Ministry of Education, Youth and Sports in the framework of the National Sustainability Programme I. All the evaluated data are available as supplementary material upon request to the corresponding authors.

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## Vzorová citace

MOTTET, Pierre; SKŘÍNSKÝ, Jan. Modelling of dense and neutral gas dispersions: LPG, methane and methanol. *Časopis výzkumu a aplikací v profesionální bezpečnosti* [online], 2016, roč. 9, č. 1-2. Dostupný z: <http://www.bozpinfo.cz/josra/josra-01-02-2016/gas-dispersions.html>. ISSN 1803-3687.

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