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MATHEMATICAL AND EXPERIMENTAL MODELLING OF AMMONIA DISPERSION BY VAPORISING AT ACCIDENT

MATEMATICKÉ A EXPERIMENTÁLNÍ MODELOVÁNÍ ŠÍŘENÍ VYPAŘUJÍCÍHO SE AMONIAKU V ATMOSFÉŘE

Abstract

In this paper, an example of mathematical modelling of ammonia dispersion in atmosphere is presented. Liquid Ammonia was spilt aground. Liguid Ammonia began vaporize promptly. Transport of ammonia was determined in different distances from ammonia source. Experiment was created by University of Defence in military area in Vyškov. Mathematical model was created in Fluent 6.3 software and was solved by finite volume method.

Abstrakt

V článku je prezentován příklad matematického modelování šíření amoniaku v atmosféře spolu s experimentem. Na zemský povrch byl rozlit kapalný amoniak, který se okamžitě začal vypařovat. V různých vzdálenostech od zdroje šíření byl stanoven transport tohoto amoniaku. Experiment byl vytvořen Univerzitou obrany ve vojenském prostoru ve Vyškově. Pro matematické modelování šíření amoniaku byl využit software Fluent 6.3. Model byl řešen metodou konečných objemů.

1 INTRODUCTION

The main reason of ammonia origin is microbial decomposition of the organic rest, excrements and animal urine. Specially agricultural production and agricultural technology escalate the concentration of ammonia in atmospheric boundary layer. In terms of technological risk, places in which ammonia concentration exceeds tolerable limits, exist. Possible accidental release can cause risk to health or can evoke property or environment damage. These places are mainly situated in industrial zone (e.g. cooling medium, dissolvent etc.), but exist in populated territory (ice pool). Because experiments in many of these places can not be realized, transport of ammonia is simulated in suitable places. Obtained knowledge is applied to real situations, [1], [4].

In this paper is presented example of mathematical modelling of ammonia dispersion in atmosphere and comparison of results of mathematical model and experiment.

Ammonia dispersion was solved in Fluent as a mixture model of turbulent flow. Mixture consisted of aid and ammonia.

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2 MATHEMATICAL MODEL OF TURBULENCE FOR COMPRESSIBLE FLOW

Turbulen*t* k-ε model was used for solving of mathematical model, which consists of following equations, [3]:

continuity equation

$$\frac{\partial\rho}{\partial t}+\frac{\partial\left(\rho\overline{u_j}\right)}{\partial x_j}=0\,, \tag{1}$$

momentum equation (Navier-Stokes equation)

$$\frac{\partial\left(\rho\overline{u}_i\right)}{\partial t}+\frac{\partial\left(\rho\overline{u_i}\,\overline{u_j}\right)}{\partial x_j}=-\frac{\partial\overline{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\left(\mu+\mu_t\right)\frac{\partial\overline{u}_i}{\partial x_j}\right)+\rho\delta_{i3}g+\rho f_c\varepsilon_{ij3}\overline{u_j}+\rho f_i\,, \tag{2}$$

energy equation

$$\frac{\partial}{\partial t}\left(\rho\overline{E}\right)+\frac{\partial}{\partial x_j}\left(\rho\overline{u_j}\overline{E}\right)=\frac{\partial\overline{p}}{\partial t}+\rho\overline{u_j}f_j+\frac{\partial\left(\tau_{jl}\overline{u_j}\right)}{\partial x_l}+\frac{\partial}{\partial x_j}\left(\lambda_{eff}\frac{\partial\overline{T}}{\partial x_j}\right), \tag{3}$$

species transport equation

$$\frac{\partial}{\partial t}\left(\rho\overline{Y}_i\right)+\frac{\partial}{\partial x_j}\cdot\left(\rho\overline{u}_j\overline{Y}_i\right)=-\frac{\partial}{\partial x_i}\cdot J_{ij}+R_i+S_i\,, \tag{4}$$

evaporizations equation

$$N_i=k_c\left(C_{i,s}-C_{i,\infty}\right), \tag{5}$$

transport equation for kinetic turbulent energy

$$\frac{\partial\left(\rho k\right)}{\partial t}+\frac{\partial\left(\rho\overline{u_j}k\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\cdot\frac{\partial k}{\partial x_j}\right)+\mu_t\left(\frac{\partial\overline{u}_j}{\partial x_l}+\frac{\partial\overline{u}_l}{\partial x_j}\right)\frac{\partial\overline{u}_l}{\partial x_j}-g_j\frac{\mu_t}{\rho\sigma_h}\frac{\partial\rho}{\partial x_j}-\rho c_d\frac{k^{3/2}}{l}\,, \tag{6}$$

dissipation rate equation

$$\frac{\partial\left(\rho\varepsilon\right)}{\partial t}+\frac{\partial\left(\rho\overline{u_j}\varepsilon\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\cdot\frac{\partial\varepsilon}{\partial x_j}\right)+\rho c_{1\varepsilon}\left(\mu_t\left(\frac{\partial\overline{u}_j}{\partial x_l}+\frac{\partial\overline{u}_l}{\partial x_j}\right)\frac{\partial\overline{u}_j}{\partial x_l}-c_{3\varepsilon}g_j\frac{\mu_t}{\rho\sigma_h}\frac{\partial\rho}{\partial x_j}\right)-\rho c_{2\varepsilon}\frac{\varepsilon^2}{k}\,, \tag{7}$$

where:

i, j = 1, 2, 3

f_c .... – Coriolis parameter $\left[\frac{1}{s}\right]$,

f_i .... – force $\left[\mathrm{N}\right]$,

g .... – gravity acceleration $\left[\frac{\mathrm{m}}{\mathrm{s}^2}\right]$,

k ..... – kinetic turbulent energy $\left[\frac{\mathrm{m}^2}{\mathrm{s}^2}\right]$,

k_c ... – mass transfer coefficient $\left[\frac{\mathrm{m}}{\mathrm{s}}\right]$,

l ...... – lenght scale of turbulence $\left[\mathrm{m}\right]$,

$\bar{p}$ ... – pressure $[\mathrm{Pa}]$,

t ...... – time $[\mathrm{s}]$,

$\overline{u_i}$ ... – velocity $\left[\frac{\mathrm{m}}{\mathrm{s}}\right]$,

x_i ..... – coordinate $[\mathrm{m}]$,

$C_{i,s}$. – vapour concentration at the droplet surface $\left[\frac{\mathrm{kmol}}{\mathrm{m}^3}\right]$,

$C_{i,\infty}$ – vapour concentration in the bulk gas $\left[\frac{\mathrm{kmol}}{\mathrm{m}^3}\right]$,

$\bar{E}$ ... – energy $\left[\frac{\mathrm{J}}{\mathrm{kg}}\right]$,

J_i ..... – diffused flux of species i $[\text{-}]$,

N_i ... – molar flux of vapor $\left[\frac{\mathrm{kmol}}{\mathrm{m}^2.\mathrm{s}}\right]$,

R_i .... – net rate of production of species i $\left[\frac{\mathrm{kg}}{\mathrm{m}^3.\mathrm{s}}\right]$,

S_i ..... – source of dispersed phase i defined by the user $\left[\frac{\mathrm{kg}}{\mathrm{m}^3.\mathrm{s}}\right]$,

$\overline{Y}_i$ ... – mass fraction of species i $[\text{-}]$,

δ_{i3} .. – Kronecker delta $[\text{-}]$,

ε .... – dissipation rate $\left[\frac{\mathrm{m}^2}{\mathrm{s}^3}\right]$,

ε_{ij3} .. – unit tensor $[\text{-}]$,

λ_{eff} –coefficient of efficient heat conductivity $\left[\frac{\mathrm{W}}{\mathrm{m.K}}\right]$,

μ ... – dynamic viscosity $[\mathrm{Pa.s}]$,

μ_t ... – turbulent viscosity $\left[\frac{\mathrm{kg}}{\mathrm{m.s}}\right]$,

ρ .... –density $\left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$,

σ_h .. – Prandtl turbulent number $[\text{-}]$,

σ_k , σ_ε , $c_{1\varepsilon}$, $c_{2\varepsilon}$, $c_{3\varepsilon}$, c_d – empirical constants $[\text{-}]$,

τ_{jl} ... – tensor of viscous tension $[\mathrm{Pa}]$,

3 EXPERIMENT

Measurement of ammonia dispersion in military area in Vyškov was made [5]. Pressure cylinder was used as a source of ammonia, see **Fig. 1**. Liquid ammonia outflow from pipe of pressure cylinder to aground and began vaporize promptly. Vapor Ammonia mass was catch by taking places (sampler), which can see in **Fig. 2**.

Fig. 1 Ammonia gas dispersion from pressure cylinder

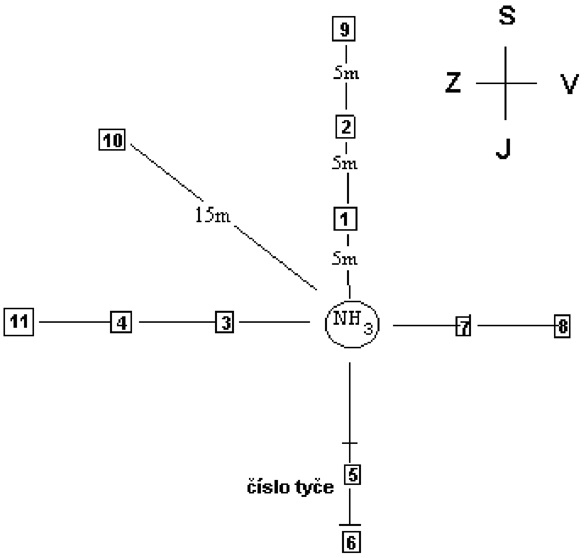

Fig. 2 Rods with taking places

Taking places consisted of filter-paper impregnated with citric acid, which reacted with ammonia gas molecules. Ammonia absorbed in sampler was determined photometricaly by the Nessler reagent, [4].

Two taking places were on one rod in every measurement, one in high 0,75 m , other 1,5 m. 3,6 kg of ammonia were released from the pressure cylinder per 10 min. Taking places were chosen in high of direct influence to humen organism.

4 MATEMATICAL MODEL

Ammonia dispersion was modeled by finite volume metod in Fluent 6.3. Firstly computational area and its grid were created in software Gambit, see **Fig. 3**. Number of cells was 736 411. The area was exported from Gambit into Fluent 6.3, where the problem was solved by $k-\varepsilon$ model. Boundary condition of velocity-inlet was set in place, where air entered into area. Air was set by velocity wind profile and direction of propagation. Velocity of liquid amonia was calculated from the required value of mass of amonia, time of distribution and diameter of pipe. Liguid Ammonia began vaporize promptly, which passes from physical properties and chemical properties, [4].

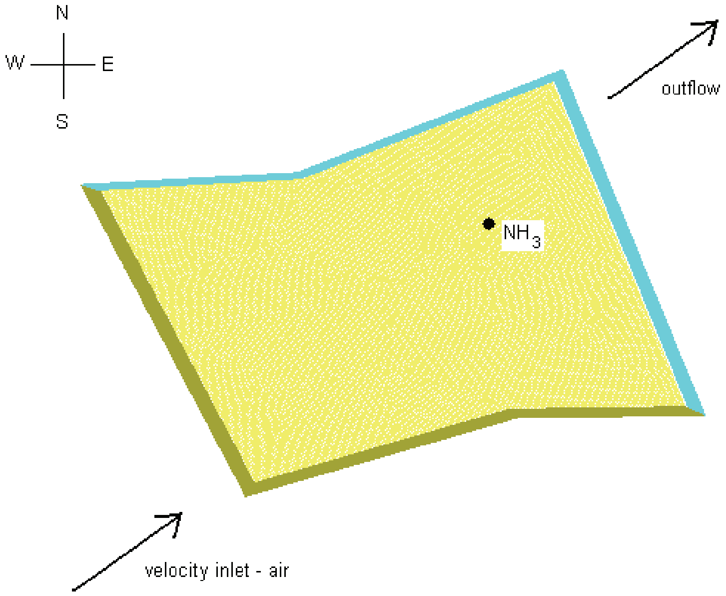

Fig. 3 Computational area

Properties of air, vapour ammonia and liguid ammonia:

Air	**vapour ammonia**	**liquid ammonia**
$\rho = 1{,}225 \left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$	$\rho = 610 \left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$	$\rho = 0{,}6894 \left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$
$c_p = 1006{,}43 \left[\frac{\mathrm{J}}{\mathrm{kg.K}}\right]$	$c_p = 4758 \left[\frac{\mathrm{J}}{\mathrm{kg.K}}\right]$	$c_p = 2158 \left[\frac{\mathrm{J}}{\mathrm{kg.K}}\right]$
$\mu = 1{,}7894 * 10^{-5} \left[\frac{\mathrm{kg}}{\mathrm{m.s}}\right]$	$\mu = 1{,}015 * 10^{-5} \left[\frac{\mathrm{kg}}{\mathrm{m.s}}\right]$	$h = 137120 \left[\frac{\mathrm{J}}{\mathrm{kg}}\right]$
$\lambda = 0{,}0242 \left[\frac{\mathrm{W}}{\mathrm{m.K}}\right]$,		

where:

c_p – specific heat capacity $\left[\frac{\mathrm{J}}{\mathrm{kg.K}}\right]$,

h – latent heat $\left[\frac{\mathrm{J}}{\mathrm{kg}}\right]$.

5 RESULTS

Concentratrations of ammonia was determined in taking places. Resultant values are listen in **Tab. 1**.

Tab. 1 Results of experiment

Taking places	concentration in 0,75 m above ground $[\mathrm{mg}\cdot\mathrm{m}^{-3}]$		concentration in 1,5 m above ground $[\mathrm{mg}\cdot\mathrm{m}^{-3}]$	
	experiment	math. model	experiment	math. model
1	4,676	27,112217	3,28	24,436449
2	2,543	10,771792	1,72	10,901752
3	1,149	4,4594064	1,97	5,2883439
4	0,985	1,1814991	0	1,2148296
5	0,411	4,5229492	2,3	4,781527
6	1,231	1,1530337	1,23	1,2323776
7	0,493	21,725393	0,41	21,069023
8	0,739	9,4273787	5,99	9,8372154
9	3,774	7,2626467	1,31	7,4929414
10	2,051	1,3773919	3,28	1,4923433
11	3,2	0,36637461	0,16	0,41289219

Hurting concentration of ammonia answers to 360 $\mathrm{mg}\cdot\mathrm{m}^{-3}$ and is red coloured in **Fig. 4**. Ammonia concentration of 15 $\mathrm{mg}\cdot\mathrm{m}^{-3}$ is displayed as transparent red colour in **Fig. 4**.

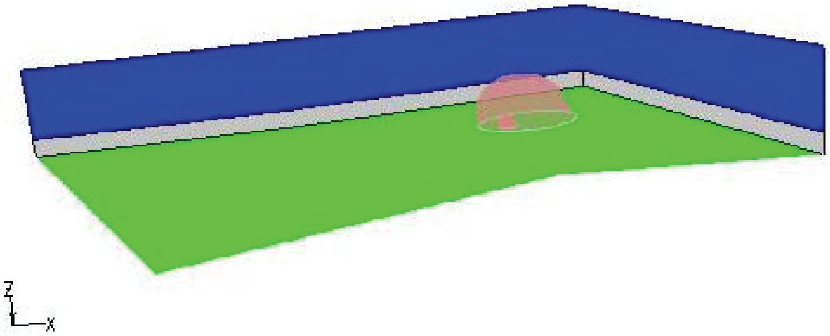

Fig. 4 Concentration of ammonia

Transport of ammonia, which was influenced with wind speed and configuration of ground is shown in plane , which is situated between 0,75 m and 1,5 m above ground, see in **Fig. 5**.

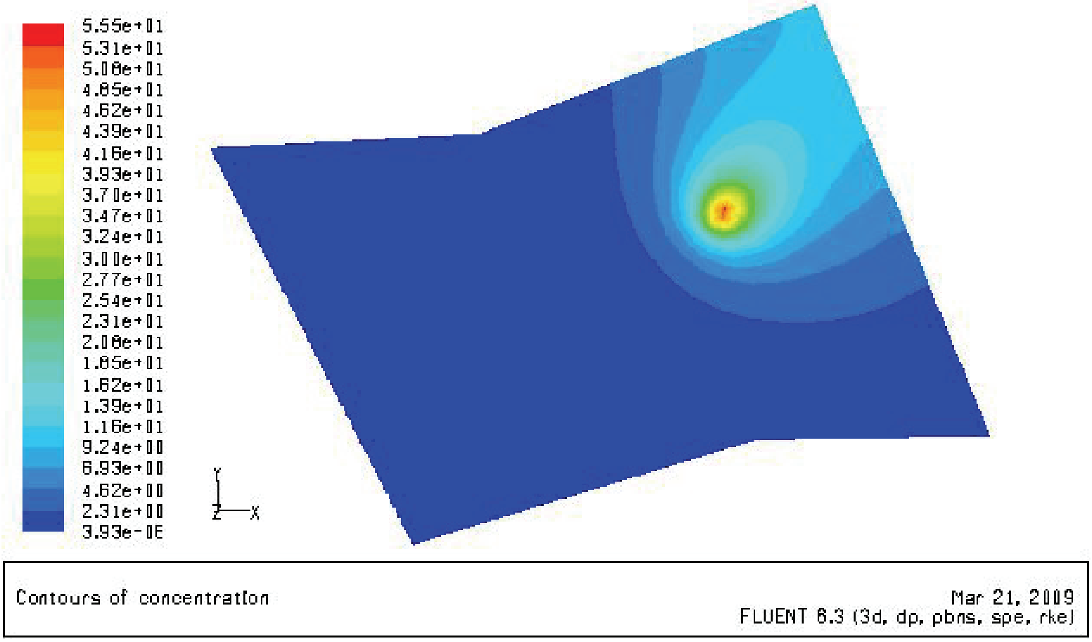

Fig. 5 Transport of ammonia

CONCLUSION

Values of amonia concentrations were in some taking places little different. These differences between experimental values and values of mathematical model were caused by several factors. One of factors was wind profile. In mathematical model wind widen only in one direction and was not changed depending on position in terrain and time. Turbulence affected the concentrations very much too. The value of kinetic turbulent energy, which was set in mathematical model, was $3{,}2\ m^2.s^{-2}$. This value was experimentally determined, [1].

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