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Josef DOBEŠ^{*}, Milada KOZUBKOVÁ^{}****MODELLING OF CAVITATION OF WASH-OUT WATER, AMMONIA WATER, AMMONIA WATER WITH INCREASED CONTENT AMMONIA AND HYDROGEN SULPHIDE, TAR CONDENSATE****MODELOVÁNÍ KAVITACE VYPÍRACÍHO ROZTOKU, ČPAVKOVÉ VODY, ČPAVKOVÉ VODY SE ZVÝŠENÝM OBSAHEM ČPAVKU A HYDROGEN SULFIDU, DEHTOVÉHO KONDENZÁTU****Abstract**

The aim is to design and implement a procedure of numerical modelling of cavitation of working mixtures: wash-out water, ammonia water, ammonia water with an increased content of hydrogen sulphide and ammonia, tar condensate. The numeric modelling is designed in the program Ansys Fluent using Schnerr-Sauer cavitation model. The issue of these liquids modelling can be solved by the cavitation simulation of water admixtures. Working fluids contain the following main ingredients: water, ammonia, carbon dioxide and hydrogen sulphide. Subsequently, a comparison of the amount of water vapor (reference liquid) and given fluid vapor is executed. The Schnerr-Sauer model is chosen because of good results in previous simulations for water cavitation. As a geometry is selected Laval nozzle. Modelled liquid mixtures are used in the petrochemical industry, as a filling for fluid circuits where cavitation may occur and therefore the research is needed.

Abstrakt

Cílem je navrhnout postup a provést numerické modelování kavitace pracovních směsí: vypíracího roztoku, čpavkové vody, čpavkové vody se zvýšeným obsahem čpavku a hydrogenu sulfidu, dehtového kondenzátu v programu Ansys Fluent s využitím Schnerr-Sauer kavitačního modelu. Problematiku modelování těchto kapalin je možno řešit simulací kavitace jednotlivých příměsí daného roztoku. Pracovní kapaliny obsahují tyto hlavní příměsi: vodu, amoniak, oxid uhličitý a hydrogen sulfid. Následně je provedeno porovnání množství páry vody (referenční tekutina) a páry zadaných tekutin. Schnerr-Sauer model je vybrán z důvodu dosažení dobrých výsledků při dřívějších simulacích pro vodní kavitaci. Jako geometrie je vybrána Lavalova dýza. Modelované směsi kapalin se užívají v petrochemickém průmyslu, jako náplň do tekutinových obvodů, kde se může vyskytnout kavitace a proto je tento výzkum potřebný.

1 NUMERICAL MODEL

The basic relation for the numerical modelling of the cavitation process (cavitation bubbles) is Rayleigh-Plesset equation [6], [7] given by the term:

$$\frac{p_{\text{vap}}(t) - p_{\infty}(t)}{\rho_{\text{LIQ}}} = R \cdot \frac{d^2 R}{dt^2} + \frac{3}{2} \cdot \left(\frac{dR}{dt} \right)^2 + \frac{4 \cdot v_{\text{LIQ}}}{R} \cdot \frac{dR}{dt} + \frac{2 \cdot \sigma_s}{\rho_{\text{LIQ}} \cdot R} \quad (1)$$

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where:

$p_{VAP}(t)$ – pressure of saturated vapor of the given liquid [Pa],

$p_{\infty}(t)$ – ambient pressure (liquid) [Pa],

ρ_{LIQ} – density of the liquid $\left[\frac{\text{kg}}{\text{m}^3}\right]$,

R – bubble radius [m],

ν_{LIQ} – kinematic viscosity of the liquid $\left[\frac{\text{m}^2}{\text{s}^1}\right]$,

σ_S – surface tension of the liquid [N.m].

This equation describes the pressure of the saturated vapor p_{VAP} and radius of the bubble R as time dependent values. Disregarding the last two members (a member of viscous and surface tension member describing the bubble) and subsequent first order approximation, an equation which is solved for a known fluid pressure $p_{\infty}(t)$ is obtained. After these modifications the final Rayleigh-Plesset equation, which describes time dependent bubble radius R [6], [7], is given:

$$\frac{dR}{dt} = \sqrt{\frac{2}{3} \cdot \frac{p_{vap}(t) - p_{\infty}(t)}{\rho_{LIQ}}} \quad (2)$$

At the multiphase cavitation flow modelling the foundation is formed by the two-phase cavitation model consisting of the standard equations of viscous flow controlling mixture transfer (Mixture model) and the general turbulence model (k- ϵ model). The continuity equation for the mixture has the form:

$$\frac{\partial \rho_{MIX}}{\partial t} + \nabla \cdot (\rho_{MIX} \overrightarrow{u_{MIX,J}}) = 0 \quad (3)$$

where:

MIX – index denoting the mixture [-],

$\overrightarrow{u_{MIX,J}}$ – mean velocity vector of mixture $\left[\frac{\text{m}}{\text{s}^1}\right]$

ρ_{MIX} – density of the mixture $\left[\frac{\text{kg}}{\text{m}^3}\right]$ of n -phases defined by:

$$\rho_{MIX} = \sum_{K=1}^n \alpha_K \cdot \rho_K \quad (4)$$

where:

K – index denoting generally the k -th phase of the mixture [-],

ρ_K – density of the k -th phase $\left[\frac{\text{kg}}{\text{m}^3}\right]$,

α_K – volume fraction of the k -th phase [1], where the volume fraction is defined:

$$\alpha_K = f_K \cdot \frac{\rho_{MIX}}{\rho_K} \quad (5)$$

Mass transfer between a liquid and a vapor or evaporation and condensation is given by the transport equation, or the equation of continuity for vapor [19]:

$$\frac{\partial}{\partial t}(\alpha_{VAP} \cdot \rho_{VAP}) + \nabla \cdot (\alpha_{VAP} \rho_{VAP} \overrightarrow{u_{VAP}}) = R_e - R_c \quad (6)$$

where:

VAP – index denoting the vapor phase [-],

α – volume fraction of the vapor [1],

$\overrightarrow{u_{VAP}}$ – mean velocity vector of the vapor phase $\left[\frac{m}{s^1} \right]$,

R_e – source term of evaporation $\left[\frac{kg}{s^1 \cdot m^3} \right]$,

R_c – source term of condensation $\left[\frac{kg}{s^1 \cdot m^3} \right]$.

1.1 Schnerr-Sauer cavitation model

For modelling of the cavitation phenomena the Schnerr-Sauer model. It defines exactly the term for a positive mass transfer from a liquid to a vapor (evaporation). The equation describing the volume fraction of the vapor in the basic case is [19]:

$$\frac{\partial}{\partial t}(\alpha_{VAP} \cdot \rho_{VAP}) + \nabla \cdot (\alpha_{VAP} \rho_{VAP} \overrightarrow{u_{VAP}}) = \frac{\rho_{VAP} \cdot \rho_{LIQ}}{\rho_{MIX}} \cdot \frac{d\alpha}{dt} \quad (7)$$

where:

VAP – index denoting the vapor phase [-],

LIQ – index denoting the liquid phase [-],

MIX – index denoting the liquid and the vapor phase - mixture [-].

The term on the right side presents the positive source term of mass transfer. The model makes use of term which marks dependence between volume fraction of the vapor α_{VAP} and the bubble number density n_B [19]:

$$\alpha_{VAP} = \frac{n_B \cdot \frac{4}{3} \cdot \pi \cdot R_B^3}{1 + n_B \cdot \frac{4}{3} \cdot \pi \cdot R_B^3} \quad (8)$$

where:

n_B – presents density of the cavitation nozzles in the fluid $\left[\frac{1}{m^3} \right]$,

R_B – radius of the bubble [m].

The general equation for mass transfer velocity $R_{e,c}$ is [19]:

$$R_{e,c} = \frac{\rho_{VAP} \cdot \rho_{LIQ}}{\rho_{MIX}} \cdot \alpha_{VAP} \cdot (1 - \alpha_{VAP}) \cdot \frac{3}{R_B} \cdot \sqrt{\frac{2}{3} \cdot \frac{P_{vap}(t) - P_{\infty}(t)}{\rho_{LIQ}}} \quad (9)$$

The radius of bubble R_B is given by next equation [19]:

$$R_B = \left(\frac{\alpha_{VAP}}{1 - \alpha_{VAP}} \cdot \frac{3}{4 \cdot \pi} \cdot \frac{1}{n_B} \right)^{\frac{1}{3}} \quad (10)$$

The substitution of the equation (6) into the equation (7) on the right side and following form by approved derivation the dependences for source terms R_e , R_c are acquired.

- if $p_{VAP} \geq p$ – evaporation starts and the source term of evaporation R_e is:

$$R_e = \frac{\rho_{VAP} \cdot \rho_{LIQ}}{\rho_{MIX}} \cdot \alpha_{VAP} \cdot (1 - \alpha_{VAP}) \cdot \frac{3}{R_B} \cdot \sqrt{\frac{2}{3} \cdot \frac{p_{vap}(t) - p_{\infty}(t)}{\rho_{LIQ}}} \quad (11)$$

- if $p_{VAP} \leq p$ – condensation starts, so the source term of condensation R_c has the form:

$$R_{e,c} = \frac{\rho_{VAP} \cdot \rho_{LIQ}}{\rho_{MIX}} \cdot \alpha_{VAP} \cdot (1 - \alpha_{VAP}) \cdot \frac{3}{R_B} \cdot \sqrt{\frac{2}{3} \cdot \frac{p_{\infty}(t) - p_{vap}(t)}{\rho_{LIQ}}} \quad (12)$$

2 NUMERICAL MODELLING OF CAVITATION OF MIXTURES IN LAVAL NOZZLE

In first stage of these modelling it is needed to compile the cavitation mechanism of the separate mixtures and modelling several infusions of the given mixtures in compliance with the task. The geometry is selected by the Laval nozzle. The input boundary conditions are as follows: mass flow rates of infusions and mixture by the mole fraction of the whole when their sum must to be equal to $3 \left[\frac{\text{kg}}{\text{s}} \right]$ (it is based on the modelling of water cavitation). It is also necessary to define other boundary conditions of the Schnerr-Sauer cavitation model.

2.1 Geometry and modelled area grid

The geometry is the selected Laval nozzle with dimensions as illustrated in the Figure 1. The Laval nozzle itself comes from an experimental facility to simulate water cavitation. For the simulation the geometry is taken with a grid already made [8], the number of the cells is 61 610.

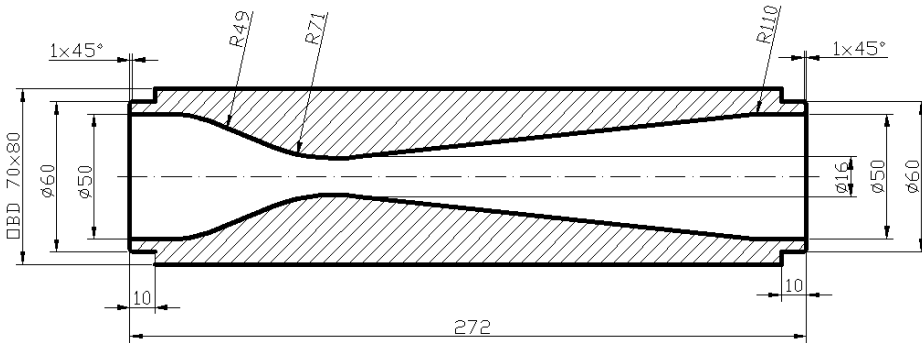


Fig. 1 The scheme of Laval nozzle [5]

2.2 Modelled liquids

The goal is to compare the amount of excreted vapor in the Laval nozzle at 30 °C for these liquids:

- Water (reference liquid),
- Wash-out water,

- Ammonia water,
- Ammonia water with an increased content of ammonia and hydrogen sulphide, called saturated water,
- Tar condensate.

Water and the corresponding water vapor are determined by the physical properties [4], [16]:

Tab. 1 Physical properties – water and water vapor

Substance	$\rho_i \left[\frac{\text{kg}}{\text{m}^3} \right]$	$\mu_i \text{ [Pa.s]}$	$p_{VAP30st} \text{ [Pa]}$	$n_B \left[\frac{1}{\text{m}^3} \right]$
H ₂ O - liquid	995,61	0,0007974	4220	1,99.10 ⁹
H ₂ O - vapor	0,030415	0,00001		

Other liquids are given by the related physical properties [10]:

Tab. 2 Physical properties –other modelled liquids

Liquid	$\rho_i \left[\frac{\text{kg}}{\text{m}^3} \right]$	$\mu_i \text{ [Pa.s]}$
Wash-out water (WW)	1030	0,00095
Ammonia water (NH ₃)	1000	0,0008
Saturated water (NH ₃ +NH ₃ +H ₂ S)	1020	0,001235
Tar condensate (TCA)	1200	0,001235
Tar condensate (TCB)	1020	0,001235

Note: Tar condensate is divided into two solutions, which differ in density ρ . The increased density (TCA) occurs when drawing the lower layer of tar.

Each mixture consists of additives; these additives will be evaporated during cavitation with the water vapor. From the available data of mass concentrations c_{wi} [10] there are the selected the additives which are present in much higher concentrations than the other substances in all investigated solutions. They are the following:

- H₂O – water,
- NH₃ – ammonia,
- CO₂ – carbon dioxide,
- H₂S – hydrogen sulphide.

In the following tables the physical properties of the pure mixed substances are presented; the water properties are already mentioned in the Table 1.

Tab. 3 Physical properties – ammonia and ammonia vapor [1], [13]

Substance	$\rho_i \left[\frac{\text{kg}}{\text{m}^3} \right]$	$\mu_i \text{ [Pa.s]}$	$p_{VAP30st} \text{ [Pa]}$
NH ₃ - liquid	595,17	0,0001283	1167200
NH ₃ - vapor	9,0533	0,000009953	

Tab. 4 Physical properties – carbon dioxide and carbon dioxide vapor [2], [14]

Substance	$\rho_i \left[\frac{\text{kg}}{\text{m}^3} \right]$	$\mu_i \text{ [Pa.s]}$	$p_{VAP30st} \text{ [Pa]}$
CO ₂ - liquid	593,31	0,000043768	7213700
CO ₂ - vapor	345,1	0,00002517	

Tab. 5 Physical properties – hydrogen sulfide and hydrogen sulphide vapor [3], [15]

Substance	$\rho_i \left[\frac{\text{kg}}{\text{m}^3} \right]$	$\mu_i \text{ [Pa.s]}$	$p_{VAP30st} \text{ [Pa]}$
H ₂ S - liquid	762,48	0,000013	2275600
H ₂ S - vapor	38,341	0,000014085	

2.3 Cavitation mechanism

The program Ansys Fluent uses the basic cavitation mechanism capable to model the transmission of only one liquid to the vapor and vice versa. Therefore here is applied a modelling approach in parts, which model each ingredient of the mixture separately. Graphically, it is possible to introduce this approach subsequently:

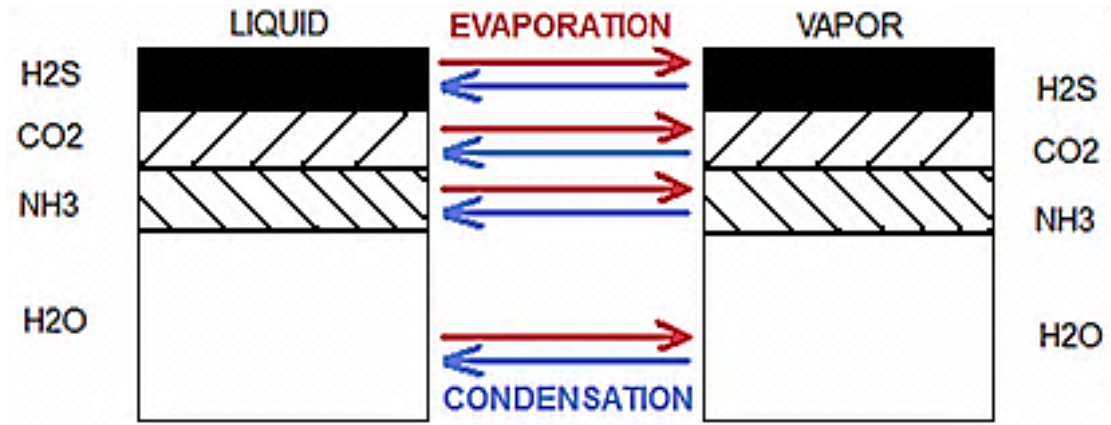


Fig. 2 The scheme of cavitation mechanism

2.3 Boundary conditions

The boundary conditions at the input are defined in terms of the mass flow of the ingredients in the mixture. To calculate the mass flow rate it is needed to calculate the mass fractions of admixtures x_{M-i} . As an example the calculation of the mass fraction x_{M-NH_3} of admixture NH₃ in the Wash-out water is given:

$$x_{M-NH_3} = \frac{c_{W-NH_3}}{c_{W-NH_3} + c_{W-H_2O}} = \frac{10}{10+10105} = 0,00979911[1] \quad (13)$$

Mass fraction in the denominator presents only a mixture of admixture NH₃ and pure substance (water) and the other ingredients are neglected. To calculate mass fraction (NH₃, CO₂, H₂S) the general form is utilized (13). The calculation of the mass fraction x_{M-H_2O} of admixture H₂O in Wash-out water is:

$$x_{M-H_2O} = 1 - x_{M-NH_3} - x_{M-CO_2} - x_{M-H_2S} = 1 - 0,009799 - 0,008342 - 0,000989 = 0,98087[1] \quad (14)$$

Tab. 6 Mass fraction of Wash-out water

Substance	$c_{wi} \left[\frac{\text{kg}}{\text{m}^3} \right]$	$x_{M-i} [1]$
Wash-out water - Σ	1030	1
H ₂ O	1010,5	0,98087074
NH ₃	10	0,009799118
CO ₂	8,5	0,008341511
H ₂ S	1	0,000988631

Following the same procedure the mass fractions of other liquid's ingredients are evaluated. They are given numerically in the literature [9]. The calculated value of the mass fraction x_{M-i} is used to define the mass flow Q_M of the substance at input. For pure water (reference liquid) the value of the mass flow Q_M is equal to $3 \left[\frac{\text{kg}}{\text{s}^1} \right]$. Further, an example of mass flow rate calculation of admixtures Q_{M-NH_3} and Wash-out water Q_{M-VR} is given:

$$Q_{M-NH_3} = 3 \cdot x_{M-NH_3} = 3 \cdot 0,009799118 = 0,02940 \left[\frac{\text{kg}}{\text{s}^1} \right] \quad (15)$$

$$Q_{M-VR} = 3 \cdot (1 - x_{M-NH_3}) = 3 \cdot (1 - 0,009799118) = 2,9706 \left[\frac{\text{kg}}{\text{s}^1} \right] \quad (16)$$

Tab. 7 The overview of mass flow rates on the input $\left[\frac{\text{kg}}{\text{s}^1} \right]$

Sub.	Wash-out water		Ammonia water		Saturated water		Tar condensate A		Tar condensate B	
	Q_{M-i}	Q_{M-VR}	Q_{M-i}	Q_{M-NH_3}	Q_{M-i}	Q_{M-NR}	Q_{M-i}	Q_{M-DKA}	Q_{M-i}	Q_{M-DKB}
H ₂ O	2,943	0,057	2,973	0,027	2,894	0,106	2,955	0,045	2,947	0,053
NH ₃	0,029	2,971	0,001	2,999	0,080	2,920	0,020	2,980	0,024	2,976
CO ₂	0,025	2,975	0,026	2,974	0,026	2,974	0,021	2,979	0,025	2,975
H ₂ S	0,003	2,997	$9 \cdot 10^{-5}$	2,999	$9 \cdot 10^{-5}$	2,999	0,004	2,996	0,004	2,996

At the input for mixture phase the boundary conditions for all simulations are defined:

- turbulent kinetic energy: $k = 0,002 \left[\frac{\text{m}^2}{\text{s}^2} \right]$,
- turbulent dissipation rate $\omega = 0,05 \left[\frac{\text{m}^2}{\text{s}^3} \right]$.

At the output for all simulations the values acquired experimentally are extended:

- absolute pressure: $10500[\text{Pa}]$,
- turbulence intensity $I = 4[\%]$,
- hydraulic diameter $d = 0,05[m]$.

2.4 Schnerr-Sauer cavitation conditions

The phase separation for each simulation, when modelling cavitation of admixtures in the mixture, is following:

- the primary phases: the liquid phase of the admixture,
- the secondary phases, the vapor phase of the admixture,
- the secondary phases: the corresponding compound containing the modelled admixture.

It is needed to define mass transfer (cavitation transmission) for each simulation, i.e. evaporation of the liquid and condensation of the vapor back. For the Schnerr-Sauer model it is needed to define the following:

- the evaporating pressure - constant value [Pa],
- the number or density of cavitation nuclei $\left[\frac{1}{\text{m}^3}\right]$.

The evaporating pressure in this case is the partial pressure of the admixture, calculated from the known values of the evaporation pressure of the pure component p_{30st} [17]. Generally, it is possible to describe the calculation of the partial pressure p_{i30st} in several consecutive steps [18]:

- the molar concentration of the component c_i is given by:

$$c_i = \frac{c_{W-i}}{M_i} \quad (17)$$

where:

c_{W-i} – mass concentration of admixtures $\left[\frac{\text{g}}{\text{dm}^3}\right]$,

M_i – molar mass of admixtures $\left[\frac{\text{g}}{\text{mol}^1}\right]$.

- Mole fraction of the component x_i is given by:

$$x_i = \frac{c_i}{\sum c_i} \quad (18)$$

where:

c_i – molar concentration of admixtures $\left[\frac{\text{mol}}{\text{dm}^3}\right]$,

$\sum c_i$ – the sum of the molar concentrations of admixtures $\left[\frac{\text{mol}}{\text{dm}^3}\right]$.

- Partial pressure p_{i30st} of the component is given by:

$$p_{i30st} = x_i \cdot p_{30st} \quad (19)$$

In the tables the partial pressures p_{i30st} for wash-out water are indicated and for other mixtures they are presented in the literature [9].

Tab. 8 The partial pressures of the individual components of Wash-out water

Sub.	$M_i \left[\frac{\text{g}}{\text{mol}^1} \right]$	$p_{30st} [\text{Pa}]$	$c_{wi} \left[\frac{\text{g}}{\text{dm}^3} \right]$	$c_i \left[\frac{\text{mol}}{\text{dm}^3} \right]$	$x_i [1]$	$p_{i30st} [\text{Pa}]$
H ₂ O	18,02	4247	1010,5	56,0766	0,9859	4187
NH ₃	17,31	1167200	10	0,5777	0,0102	11855
CO ₂	44,01	7213700	8,5	0,1931	0,0034	24495
H ₂ S	34,08	2275600	0,03	0,0293	0,0005	1173
Σ	-	-	-	56,8768	1	41712

Cavitation nuclei density n_B is determined according to the literature [12] using a chart or computed according the following equation:

$$n_B = n_* \cdot \left(\frac{p_{VAP} - p_{MIN}}{p_{VAP}} \right)^{m_B} \quad (20)$$

where:

n_* – basic number of cavitation nuclei, $n_* = 2.10^{-13} \left[\frac{1}{\text{m}^3} \right]$,

p_{VAP} – vaporizing pressure [Pa],

p_{MIN} – minimum pressure, estimated separately for each simulation [Pa],

m_B – exponent for the distribution of cavitation nuclei [1], $m_B > 0$, it is chosen $m_B = 1$.

Cavitation nuclei density is in the range $1.6.10^8 \div 1.710^0 \left[\frac{1}{\text{m}^3} \right]$ for all modelled admixtures.

2.5 Experiment

Unfortunately, in this case the experiment results were not available for comparison. The reason is the high aggressiveness of the examined substances due to which it was necessary to prepare a new experimental circuit resistant to aggressive substance.

2.6 Numerical results

The mean value of the excreted vapor amount [kg] in the whole area of the Laval nozzle was calculated. The values of the steam amount [kg] are written in the Table 9:

Tab. 9 The summary of the results of the modelled vapor amount of mixtures

Vapor [kg]	Water (H ₂ O)	Wash-out water (WW)	Ammonia water (NH ₃)	Saturated water (NH ₃ +NH ₃ +H ₂ S)	Tar condensate A (TCA)	Tar condensate B (TCB)
H ₂ O	$2,8.10^{-4}$	$7,11.10^{-4}$	$4,88.10^{-4}$	$7,04.10^{-4}$	$2,74.10^{-4}$	$3,67.10^{-4}$
NH ₃	0	$4,62.10^{-5}$	$9,45.10^{-6}$	$7,76.10^{-4}$	$7,22.10^{-6}$	$3,07.10^{-5}$
CO ₂	0	$4,29.10^{-5}$	$5,66.10^{-5}$	$4,68.10^{-5}$	$1,75.10^{-5}$	$4,56.10^{-5}$
H ₂ S	0	$7,96.10^{-6}$	$1,02.10^{-5}$	$8,11.10^{-6}$	$2,56.10^{-6}$	$1,01.10^{-5}$
Σ	$2,8.10^{-4}$	$8,08.10^{-4}$	$5,64.10^{-4}$	$1,54.10^{-3}$	$3,01.10^{-4}$	$4,53.10^{-4}$

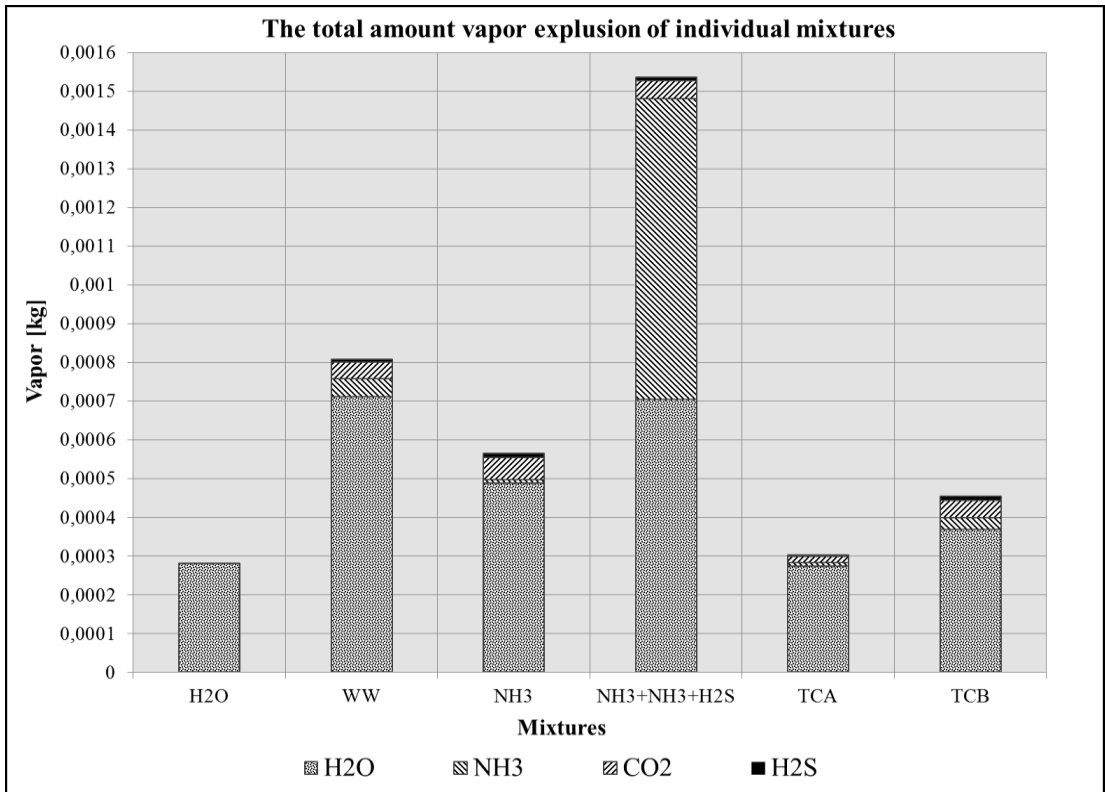


Fig. 3 A graph of the total vapor amount of individual mixtures

3 CONCLUSIONS

The Schnerr-Sauer model was selected on the basis in previous experience solving water cavitation in the Laval nozzle and also in order to achieve good results in comparison with the experiment. At the same time it allows to evaluate averaged quantities (Unsteady Statistics) of unstable processes such as cavitation. As geometry the Laval nozzle by specified dimensions was selected as illustrated in the Figure 1.

The boundary conditions are based on the numerical simulation of cavitation of pure water, this concern in particular to the total mass flow rate at the inlet and pressure at the outlet and values of turbulent quantities (the turbulent kinetic energy and the dissipation rate). The total mass flow rate at the inlet was divided into the mass flow rate of the ingredients in relation to their mass fraction. The partial pressures of mixed compounds were calculated using the mole fraction and the valorization pressure of pure ingredients.

As the graph in the Figure 3 indicates, the largest volume of vapor is seen for saturated water, which is caused primarily due to the high concentration of ammonia. The second mixture with the largest number of excluded vapor is wash-out water, closely followed by ammonia water, tar condensate and pure water. From this graph it is possible to conclude that saturated water at cavitation conditions will cause largest cavitation wear in comparison to other substances.

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