

## Modeling the impact of consequence of ammonia release from ship loading arm by CFD

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In the energy, oil, gas and petrochemical industries, all stages of mining, production, storage and material handling rely on complex and risky technologies. Always fear to multiple events, resulting in irreparable damage to human and environment seen. Release of hazardous materials in this industry, has always been one of the threatening factors. One of the most dangerous materials in the petrochemical industry is ammonia. However, Engineering and management measures are always considered for prevention of spills and releases of materials, yet often human errors in the control of unit and/or emerging process failures during the maintenance, as well as structural defects or sometimes sabotages all caused such events occur. Hence, one of the effective methods in measuring risk and therefore providing preventive measures as well as emergency management measures mentioned studying Consequences of events and forecasting pollutants and hazardous gases together with various methods. This study in initial aims to study a variety of methods provided for modeling pollutant emissions, then goes forward using computational fluid dynamic to model sudden detachment of marine loading arms during loading ship designed to transport ammonia in one of ports at South Pars in Iran located at Assaloyeh region. It should be noted this study even in terms of emission source and software is distinctive, and conducted for the first time in the world. How ammonia released, regions under influence of lethal concentrations as well as dangerous and lethal concentrations of ammonia forecasted, and suggestions to reduce financial losses have been proposed.

**Keywords:** South Pars - ammonia – ship loading arm, release of pollutants, modeling using CFD

### INTRODUCTION

Today, numerous and dangerous environmental, health and safety events arising from the emission, flammability and explosion of toxic and hazardous chemicals in various industrial units, ask for preventing and/or coping with such dangers and their different consequences as well as emergency management during these events. Ammonia is one of the hazardous substances, all units of production, storage and ammonia loading and transmission are always of the most hazardous units across Petrochemical industries. Ammonia is easily liquefied due to the strong hydrogen bonding between molecules, this gas is lighter than air, yet if emission of this substance comes to realize in liquid, due to lower temperatures and pressures, the liquid droplets and the gas particles together enter to the environment, thus acts as a heavy gas. Ammonia is

highly irritating and cause severe irritation of skin, eyes and respiratory system and cause severe damage to the lungs. High concentrations of 150 ppm have been dangerous for human, and cause death at concentrations higher than 700 ppm [1]. The stages for production, transmission and export of ammonia due to different reasons including Human error, equipment corrosion, collision of heavy objects, vandalism attacks and so forth would result in risk of ammonia release in different amounts. Hence, forecast and modeling how ammonia release and/or any other pollutant before emerging event come useful to detect the sites subjecting to emission after occurrence of event, and further detect the concentrations of chemicals in which lethal or hazardous concentrations go beyond, and then reduce environmental, financial and living damages by providing proper engineering and management measures in paradigms of emergency management and crisis management.

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In general, two methods can be considered to forecast how pollutants release. The first is the use of results from experimental and real tests. The second is the use of modeling and numerical simulations.

In this regards, Yoshihito Tominaga [2] proposed his study, mentioned that Near-field pollutant dispersion in the urban environment involves the interaction of a plume and the flow field perturbed by building obstacles. In the past two decades, micro-scale Computational Fluid Dynamics (CFD) simulation of pollutant dispersion around buildings and in urban areas has been widely used, sometimes in lieu of wind tunnel testing. Key features of near-field pollutant dispersion around buildings from previous studies, i.e., three-dimensionality of mean flow, unsteadiness of large-scale flow structure, and anisotropy of turbulent scalar fluxes, are identified and discussed. It is important to choose appropriate numerical models and boundary conditions by understanding their inherent strengths and limitations. Furthermore, the importance of model evaluation was emphasized. Because pollutant concentrations around buildings can vary by orders of magnitudes in time and space, the model evaluation should be performed carefully, while paying attention to their uncertainty. Although CFD has significant potential, it is important to understand the underlying theory and limitations of a model in order to appropriately investigate the dispersion phenomena in question. One of the first studies in which CFD used to simulate emission of gases, the studies by [3] can be mentioned, that they used  $k-\epsilon$  Turbulence model to consider viscosity effects of turbulence. Using these instruments faced with progress at computer hardware. Perdikaris stated in this context that computational fluid dynamics (CFD) has been recognized as a potent tool for realistic estimation of consequence of accidental loss of containment because of its ability to take into account the effect of complex terrain and obstacles present in the path of dispersing fluid. The key to a successful application of CFD in dispersion simulation lies in the accuracy with which the effect of turbulence generated due to the presence of obstacles is assessed. Hence a correct choice of the most appropriate turbulence model is crucial to a successful implementation of CFD in the modeling and simulation of dispersion of toxic and/or flammable substances. In this paper an attempt has been made to employ CFD in the assessment of heavy gas dispersion in presence of obstacles [4-6].

M.A. McBride et al. [6] stated safety reports required for sites storing quantities of dangerous substances in excess of specified levels. The safety

report should include an assessment of the risk associated with the facility, which will include an evaluation of the effects of releases of dangerous substances to the environment. The models commonly used for assessing the dispersion of dense gases in the atmosphere are based on the unobstructed terrain. They proposed physical modeling of releases in a Boundary Layer Wind Tunnel (BLWT) and the use of Computational Fluid Dynamics (CFD). Their paper focuses on the key findings of the study, which provide a dramatic insight into how terrain and buildings can fundamentally alter the dispersion behavior of dense gases. The results show how flat terrain models may overestimate the chlorine hazard range by as much as a factor of 5, whilst the predicted direction of travel of the cloud may err by up to 90. Eslam Kashi in a study entitled "Temperature Gradient and Wind Profile Effects on Heavy Gas Dispersion in Build up Area" , stated dispersion of heavy gases is considered to be more hazardous than the passive ones [7-15]. This is because it takes place more slowly. In this paper, based on the extensive experimental work of Hanna and Chang, the CFD model was tested compared with Kit Fox experiments. In order to accomplish this validation, the multiphase approach was employed as a new method in this area. In addition, the temperature gradient effects were investigated. The survey of wind speed was done taking factors such as time, height and direction into the consideration. To reduce the number of elements in computational domain, a combination of 2D and 3D geometries were utilized [16-20]. Results showed that the wind inlet correction and temperature gradient had a significant influence on gas concentration records. Alberto Mazzoldi "CFD and Gaussian atmospheric dispersion models: A comparison for leak from carbon dioxide transportation and storage facilities" stated Carbon Capture and Storage (CCS) is of interest to the scientific community as a way of achieving significant global reduction of atmospheric CO<sub>2</sub> emission in the medium term. CO<sub>2</sub> would be transported from large emission points (e.g. coal fired power plants) to storage sites by surface/shallow high pressure pipelines. Modeling of CO<sub>2</sub> atmospheric dispersion after leakages from transportation facilities will be required before starting large scale CCS projects. This paper deals with the evaluation of the atmospheric dispersion CFD tool Fluid-PANACHE against Prairie Grass and Kit Fox field experiments [21-23]. A description of the models for turbulence generation and dissipation used ( $k-3$  and  $k-1$ ) and a

comparison with the Gaussian model ALOHA for both field experiments are also outlined.

The main outcome of this work puts PANACHE among the “fit-for-purpose” models, respecting all the prerequisites stated by Hanna et al [24,25]. for the evaluation of atmospheric dispersion model performance. The average under-prediction has been ascribed to the usage of mean wind speed and direction, which is characteristic of all CFD models. The authors suggest a modification of performance ranges for model acceptability measures, within the field of high pressure CO<sub>2</sub> transportation risk assessment, with the aim of accounting for the overall simplification induced by the usage of constant wind speed and direction within CFD atmospheric dispersion models. As observed, many researchers provided a variety of studies on accuracy of different turbulence models in predicting emission. Study by Zhang et al. [13] can be remembered here. Zhang has used k-ε model to model gas emission with density over air. The results of their study to the experimental results found with acceptable error 2.2%. Currie et al. in 2012 using CFD examined how a heavy gas dispers in an area and addressed evaluating risk regarding the results.

Given the progress in software and hardware contexts particularly at the recent decade, using CFD to predict how the pollutants emit at residential and industrial areas has been increased. Indeed, CFD and/or modeling flow in a three-dimensional form is as a virtual laboratory in which effect coming from different parameters on flow can be examined easily with very low costs rather than experimental methods like real measurements. This study aimed to simulate ammonia gas emissions from at one of Iran's South Pars dock located in Asalooeye area using CFD. Such a study has not conducted to date in Iran, that this study is the first project in which this topic has been discussed. Since results of real measurements do not exist to evaluate accuracy of results from modeling ammonia emission from one of Iran's South Pars dock located in Asalooeye area, thus the experiments associated to a real sample have been used to evaluate the accuracy of the results of this project. For this, the results of Thorney Island have been used.

### THREE-DIMENSIONAL SIMULATION ALGORITHM

To simulate using CFD, the specific stages for simulation process have to be paved and such stages dependant from type and geometry are simulated, and they have shown in Fig 1.

One numerical method to resolve integral form of prevailing equations is the Finite volume or the

control volume [16]. In this method, the physical amplitude is divided to small volumes and the dependant variables are measured at the center of volumes or in corners. Equations resolving at the computational area regarding the physical conditions of field are the very Conservation equations of mass and momentum.

Further, to simulate disturbance of flow, transmission equations are resolved for turbulence flow. This study aims to achieve ammonia concentration at different times and places at computational area. Thus, species conservation equation has to be resolved at these problems. In following, a summary of these equations has been addressed.

Species conservation equation is written as follows: [17]

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad (1)$$

Where  $\rho$  and  $u_i$  are fluid density and components of average speed.

The equation of motion extent and/or momentum at direction i is written as follow: (17)

$$\begin{aligned} \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_i} (\rho u_i u_j) = \\ - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_i \end{aligned} \quad (2)$$

In expression above,  $p$ ,  $\tau_{ij}$ ,  $\rho g_i$  are static pressure, stress tensor and physical force of gravity in direction of i. in expression 2, stress tensor is defined as expression 3. In expression 3,  $\mu$  is molecular viscosity of the fluid and  $\mu_t$  is not of the features of fluid, and is defined and entitled shear viscosity in turbulent flows.

$$\tau_{ij} = \left[ \mu_{eff} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_j} \delta_{ij} \quad (3)$$

$$\mu_{eff} = \mu + \mu_t$$

Yakhot et al. [18] proposed a new type of k-ε model in which functional features and characteristics compared to standard model reported. The proposed model based on renormalized group theory reported so-called RNG. RNG k-ε model in its physical form is similar to standard model.

General form of equations at RNG k-ε is as follows:

$$\begin{aligned} \rho \frac{\partial k}{\partial t} + \rho u_j k_{,j} = & \\ \left( \mu + \frac{\mu_t}{\sigma_k} k_{,j} \right) + G + B - \rho \varepsilon & \\ \rho \frac{\partial \varepsilon}{\partial t} + \rho u_j \varepsilon_{,j} = & \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \varepsilon_{,j} \right)_{,j} \quad (4) \\ + C_1 \frac{\varepsilon}{k} G + C_1 (1 - C_3) \frac{\varepsilon}{k} B - & \\ C_2 \rho \frac{\varepsilon^2}{k} - \frac{C_\mu \eta^3 \left( 1 - \frac{\eta}{\eta_0} \right)}{1 + \beta \eta^3} \frac{\varepsilon^2}{k} & \end{aligned}$$

In equation above, the additional term contains  $\eta$  parameter, indicating characteristic time of turbulence. Characteristic time of the flow field. Hence, model of off-equilibrium effects have been also considered.

The main coefficients of model RNG for Isothermal flows include:  $\sigma_\varepsilon$ ,  $\sigma_k$ ,  $C_1$ ,  $C_2$ , and  $C_\mu$ .

Two other coefficients, that is,  $\eta_0$  and  $\beta$  using Von Karman constant  $K$  are these coefficients and obtained. The coefficients below are the ordinary coefficients used in this model.

| $\sigma_k$ | $\sigma_\varepsilon$ | $C_\mu$ | $C_1$ | $C_2$ | $K$ |
|------------|----------------------|---------|-------|-------|-----|
| 0.7        | 0.7                  | 0.      | 1.    | 1.    | 0.3 |
| 179        | 179                  | 085     | 42    | 68    | 875 |

$\eta_0$  and  $\beta$  are obtained using the coefficients below:

$$\begin{aligned} \eta_0 &= 4.38 \\ \beta &= 0.015 \end{aligned} \quad (5)$$

#### VERIFICATION OF CFD RESULTS AT THIS PROJECT

To evaluate accuracy of results, As the results for real measurements due to a specific type of Scenario for the destruction of the ship's tanks of ammonia exports do not exist, the experiments associated to a real sample have been used. For this, the results of Thorney Island experiment in this study have been used. The first phase of field experiments to spread heavy gas dispersion trials at Thorney Island associated to release of gas in an area without barrier considered, yet the second phase of experiments aimed to examine heavier gas dispersion than air in surrounding barriers [19].

In the experiments associated to a barrier, a cube 9 m × 9 m × 9 m, which was made of wood and plastic sheets the trailers for moving obstacle and put it in the proper position has been used; further, a trailer to displace barrier and place it in proper positions have been used. Gas supply cylinder (actually a 12-sided) with a diameter of 14 meters and a height of 13 m, and a volume of 2000 cubic meters reported. In this part of the project of Ammonia, Test Results for Project No. 26 Thorney Island for assessment and verification of CFD has been used [19]. In this experiment, a cube barrier in distance placed 50 meter lower than cylinder. Ga mixture containing 68.4% nitrogen and 31.6% Freon mentioned 12, that during this experiment, the wind speed has been measured approximately 1.9 m/s.

#### GEOMETRY MODELING AND NETWORKING

Computational area in this modeling considered 150m × 100m × 40m cube dimensions. Due to the geometry and the symmetry with respect to the symmetry passing through the center of the cube, the flow in symmetrical regarding boundary conditions is solved. In Fig 1, the networking has been shown.

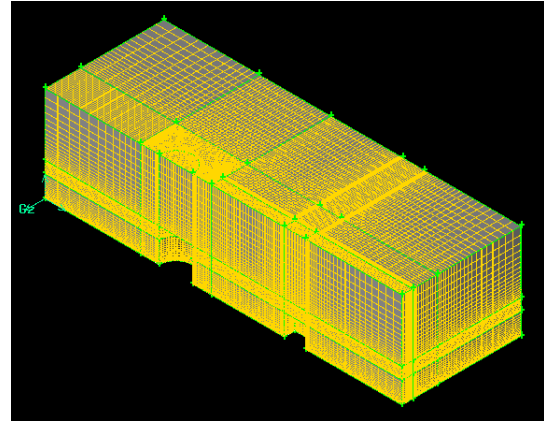


Fig 1. Networking computational field of Thorney Island.

#### APPLYING BOUNDARY CONDITIONS

##### Wind input flow

Wind speed is one of the most important factors in the spread and dilution of gas, and transmitted gas to different parts of the range. If wind speed taken in a defined height, then the speed profile using exponential expression can be expressed as follows:

$$u = u_0 \left( \frac{z}{z_0} \right)^\lambda \quad (5)$$

Where  $\lambda$  is a dimensionless value and its value relies on the extent of sustainability and also roughness of dependent surface. Given the experiment conditions No 26, values of  $\lambda$  and

roughness have been represented in Table 1 as shown below.

**Table 1.** Features of wind profile

| Wind speed at the reference height(m/s) | Roughness of surface(m) | $\lambda$ |
|---|-------------------------|-----------|
| 1.9                                     | 0.005                   | 0.07      |

*Gas input*

According to the experiment no 26, about 2000 m<sup>3</sup> of gas mixture at lower than 1.5 second is released at atmosphere to enter the boundary conditions at Transient state of mass flow rate, the gas mixture is defined through Step Function.

$$Q = m_i \cdot \text{step}[-(t - 0)(t - 1.5)] \quad (6)$$

Where  $m_i$  has been defined in Table 2.

**Table 2.** Values of  $m_i$ , mass flow and the volume of gas released

| Mass Inflow Rate (kg/s) | Total Released Mass (kg) | Total Released Volume (m3) |
|-------------------------|--------------------------|----------------------------|
| 3178                    | 4767                     | 1970                       |

*Walls*

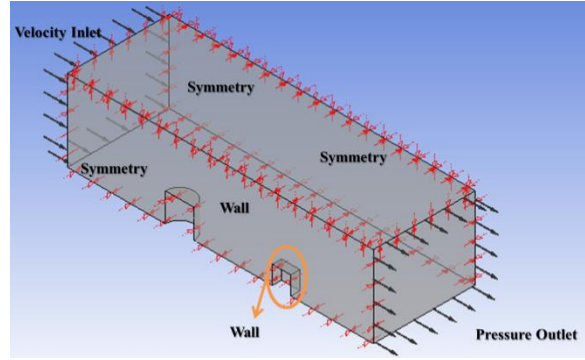
In the course of solving the steady state, barrier and cylinder are taken into account, and in the course of solving transient state, barrier with the condition of the walls is considered. Furthermore, the ground surface is specified with the wall boundary condition. To the earth surface, the roughness of surface with 0.005 meter, and to the barrier and cylinder, the supposition of the smooth surface is used.

**SYMMETRY BOUNDARY CONDITION**

As mentioned, the plane of symmetry passing through the center of the cube as the Symmetry boundary condition is considered. Furthermore, upper and lateral surfaces given that taken sufficiently far from barriers, and the flow would sustain steady at this area, are defined with Symmetry boundary condition. In general, Symmetry boundary condition causes the gradient perpendicular to the surface with different components at flow field taken equal to zero.

**OUTPUT OF FLOW**

In downstream of flow, Pressure outlet boundary condition is used. The outlet pressure is taken equal to atmospheric pressure. In Fig 2, the boundary conditions at different surfaces have been indicated.



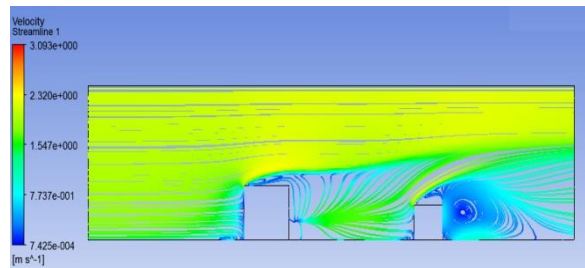
**Fig 2.** The boundary conditions acted

**RESULTS**

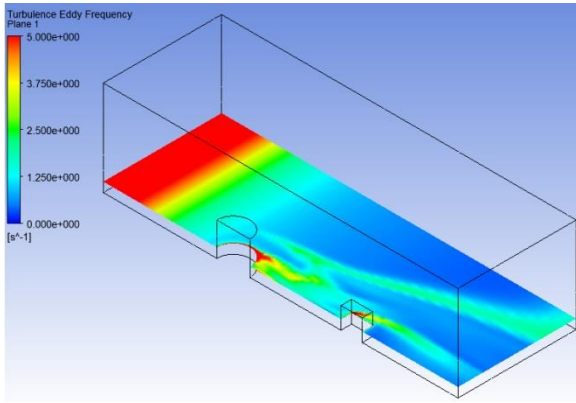
The flow in nature in this problem taken as a transient flow; to resolve transient flow, all the time considered for modeling, time steps and early conditions have to be taken as the input. To determine the early conditions, in initial the flow has to be resolved in steady state and its results have to be applied as the early conditions so as to resolve the transient flow. In initial, the results of stationary status were entered into discussion and later the results associated to the transient flow have been discussed as well.

**THE RESULTS OF STEADY FLOW**

In Fig 3, the flow lines in the plane of symmetry passing through the center at the computational area have been shown. As expected, separation of flow and building Vortices behind the barriers can be seen. In Fig 4, Eddie Cantor frequency has been shown. As observed, at most areas, this frequency placed at the area 1 Hz. As a result, the time interval for eddies at 1 second placed, that this makes the comparison between experimental results and numerical results possible.



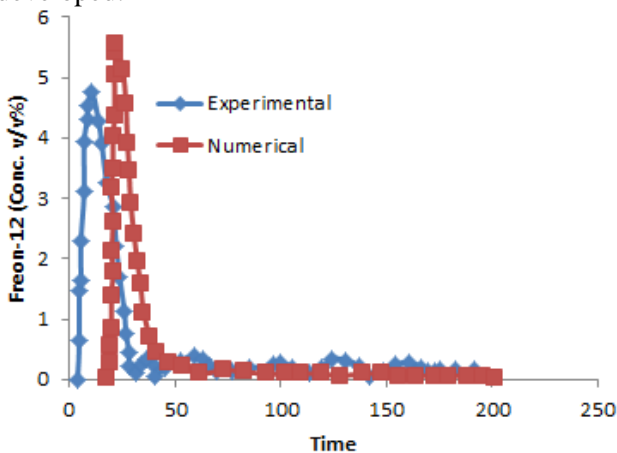
**Fig 3.** Flow lines for steady status



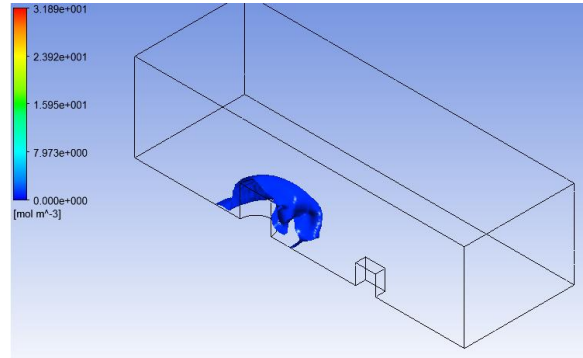
**Fig 4.** Eddie frequency disturbance.

### THE RESULTS OF THE TRANSIENT CURRENT

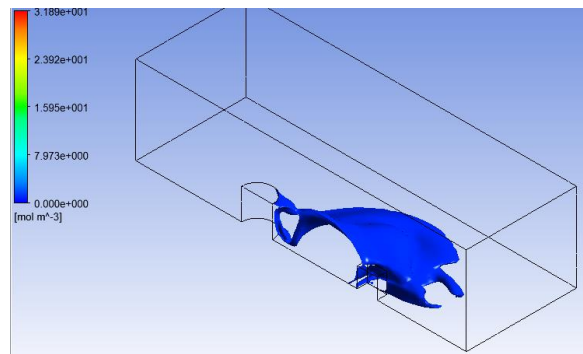
In Fig 5, the simulation results with experimental data measured at the Front part and entrance of building at the height 6.4 were compared. As observed, the results with an appropriate accuracy have estimated the process. The analytic and experimental results differ with each other in about 10 seconds, that is, the first gas concentrations at the given area at the analytic results suspected 10 seconds later. Maximum concentration at analytic results in 22.1 second with 5.42 amount has been recorded, yet this maximum concentration at the experimental results has been recorded at 11.4 second with the amount of 4.75. In Fig 6 and 7, the surfaces with the same potentials for concentration  $1 \text{ mol/m}^3$  at different time intervals have been shown. Indeed, these surfaces in terms of quantity and flammability show that risk and outcomes coming are ranked the first in the analysis computations. As observed, due to heaviness of Freon gas than air, immediately after gas released, the cloud mass in downstream and in an area close to earth is developed.



**Fig 5.** the comparison of simulation results with experimental data measured in front area of building at height 6.4.



**Fig 6.** the area with the same potential for concentration  $1 \text{ mol/m}^3$  at time  $t=4\text{s}$ .



**Fig 7.** the area with the same potential for concentration  $1 \text{ mol/m}^3$  at time  $t=50\text{s}$

In this study, computational fluid dynamic was used to simulate the sudden explosion scenario of one of ship tanks for transport and export of ammonia at one of Iran's South Pars dock located in Asalooeye area . areas under influence of Dangerous and lethal concentrations of ammonia concentration driven from predicted incident regarding the suggestions to reduce human and financial losses.

### NUMERICAL ANALYSIS OF CONSEQUENCE FROM AMMONIA RELEASE ARISING FROM DETACHMENT OF LOADING ARM IN ONE OF PORTS AT SOUTHERN PARS REGION

This study aims to provide numerical modeling for ammonia emission arising from sudden detachment of loading arm during loading in a ship designed for ammonia export in one of ports at southern pars region. The capacity of ships varied, mentioned from 15 to 40 thousand tons. Modern ships to prevent leakage are designed with two-walls. Further, due to the fact that a ship to sustain on its ability to carry different liquid products, and not losing all loaded liquids during any damage and leakage, includes several loading tanks to load pipeline containing ammonia in, loading arm is placed between pipeline and ships tanks. After producing ammonia in petrochemical unit, and

passing 1.5 km through external pipeline from Petrochemical producing ammonia, this substance liquefies entering to loading part in port.

Detachment of loading arm during ship loading operations is of hazardous events occurred in ports. In this case, a large volume of chemicals enter to the environment, and due to toxicity and reaction of the substance, many environmental effects would be resulted. Hence, modeling ammonia emission arising from detachment of loading arm during ship loading is of main objective in this project.

### GEOMETRIC NETWORKING

Dimensions of computational area have been presented in Fig 8. As shown, this computational area includes different barriers in different forms. All the structures existing around port have been modeled. The computational area includes a series of rack structures, Transmission lines of petrochemical products, two building next to each port, port and administrative buildings.

Upward perspective of port has been indicated in Fig 9, and geometric modeling for rack structures has been indicated in Fig 9. Areas shown with orange color indicate Administrative buildings.

One of the most optimized methods to reduce elements besides keeping accuracy is generating network with organization. In complex geometries, the only way to reach to this aim mentioned dividing the main geometry to smaller parts with the ability to generate network with organization within them. For this, computational area has been divided to 456 smaller parts.

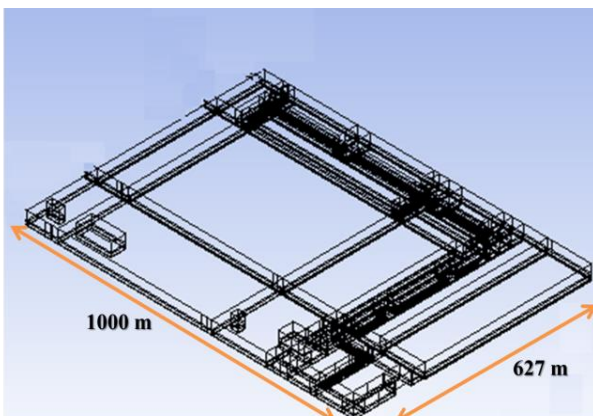


Fig 8. Dimensions of computational area.

These blocks can be seen in Fig 10. Yet, accordingly all the computational area cannot be divided to cube blocks. As a result, in the remaining areas, the only solution can be the use of disorganized network.

Thereby, blocks in which disorganized network generated, reduces. As a result, disorganized network has been generated in smaller space of

computational area. This reduces elements in substantial amount. Finally, 2893527 networks generated.

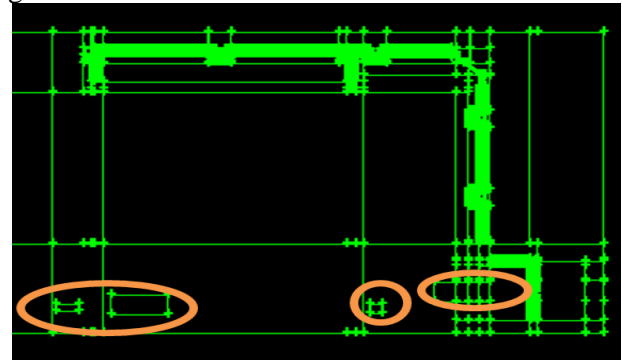


Fig 9. upward perspective of geometry and position of buildings.

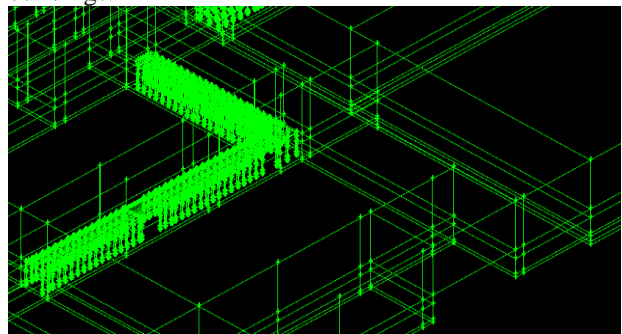


Fig 10. Geometry generated for rack structure.

### MODELING WITH USE OF CFD

According to the data through operation unit, a point which can cause leakage mentioned loading arm. Scenario defined in this part arises from sudden detachment of arm joint and ship joints during loading operations.

According to this scenario, all of a sudden joint between arm and ship removed, and ammonia release appeared. As a result, The exit of accumulated ammonia would be with flow rate about 190 kg/s for 30 seconds. Temperature for released ammonia has been mentioned 33 ° C. numerical modeling sustained on for 10 minutes. Furthermore, Environmental condition has been chosen autumn season. Wind speed has been considered 9.78 m/s, and temperature has been taken 30° C.

### APPLYING BOUNDARY CONDITIONS

#### Wind flow

According to the data about weather stations, prevailing speed has been taken 9.8 m/s. conditions applied for wind flow have been mentioned in Table 3.

Table 3. Conditions applied for wind flow entry

|                      |          |
|----------------------|----------|
| Temperature          | 30° C    |
| Wind speed           | 9.78 m/s |
| Sustainability class | D        |

|                                |          |
|--------------------------------|----------|
| Entry angel for flow to axis z | 8 degree |
| Intensity of flow disturbance  | 5%       |

#### Exit of wind flow

Boundary condition for exit pressure has been used at these levels. Adjusted pressure considered 1 atm.

#### Gas entry

To model ammonia release from loading arm, it is supposed that ammonia gas with flow rate 190 kg/s for 30 seconds due to detachment of loading arm enters to the area. This flow considered as flow passing through pipelines during loading. Furthermore, Turbulence intensity has been taken 5%. Temperature of ammonia entered to area considered  $-33^{\circ}\text{C}$ , equal to temperature of ammonia gas inside pipes.

#### Symmetry boundary condition

Upward surface at computational area placed at a height in which gradient of flow parameters taken zero. As a result, supposition to use symmetry boundary condition at this area is an acceptable supposition, that this condition considers gradient perpendicular to this surface for flow variables, about zero.

#### Wall boundary condition

All the solid surfaces existing in computational area like buildings, structures and pipes are defined with solid wall boundary condition. This condition indicates that gradient perpendicular to these surfaces is zero, that is, flow steaks to solid surfaces.

#### ADJUSTMENTS FOR CONVERGENCE

The highest length that a particle must pass from flow field from entry surface to exist surfaces equals to diameter of a surface like upward surface at computational field. The diameter considered equal to 1180 meter, assumed that this particle passes the computational area with wind speed, and as a result passing time would be 120 seconds.

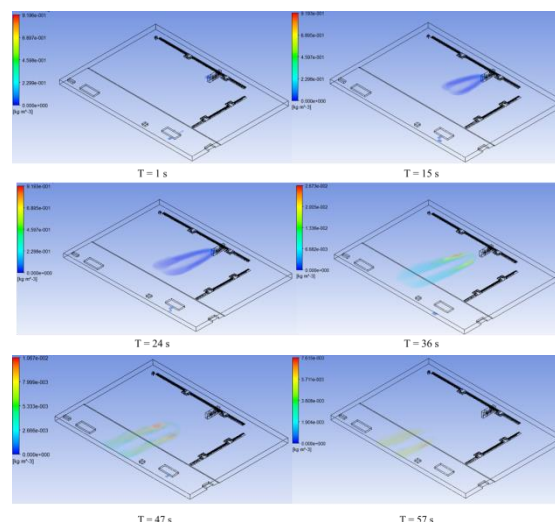
Considering time interval equal to 0.05 seconds means that a photo for 2400 times is taken of a particle in moving, that is, field equations would be resolved in passing a particle from field.

#### RESULTS

In initial, how ammonia releases in an area has been presented in three dimensions. Fig 11 indicates this fact. Rack structures in right side and administrative buildings in drought are not influenced. This goes on to 85 seconds later emission so far as ammonia cloud exits from computational area.

The most important limit to develop response program at emergency conditions is the limit in which effects of threatening individuals' life exist. The most important exposure limits used include:

- Emergency Response Planning Guideline (ERPG) belonged to American Industrial Hygiene Association
- Immediately Dangerous to Life and Health (IDLH)



**Fig 11.** Ammonia emission at computational area at different time intervals for emission from loading arm

- Threshold Limit Values (TLV) belonged to American Conference of Governmental Industrial Hygienists

ERPG exposure limit indicates the concentration that causes effects on individuals' health in compliance with the existing concentrations seen.

ERPG1: This is the maximum airborne concentration below which nearly all individuals could expose to the substance as much as one hour, without any minor and temporary adverse effect on health imposed and smell felt.

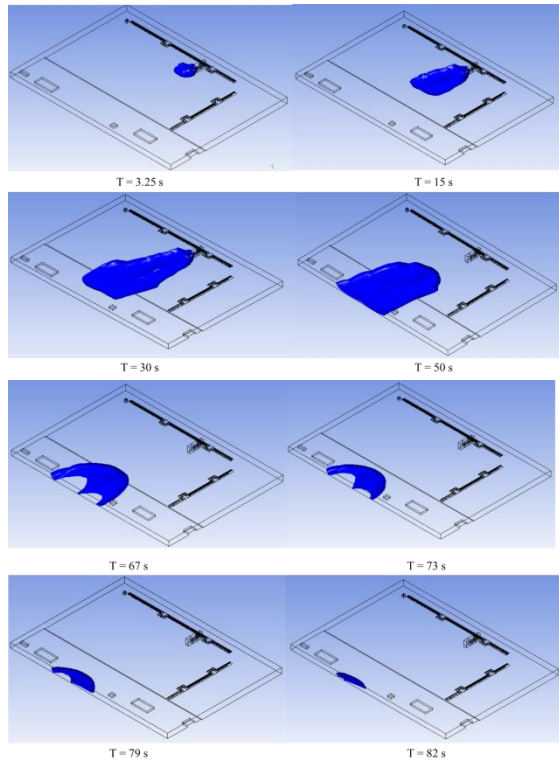
ERPG2: This is the maximum airborne concentration below which nearly all individuals could be in this area for an hour using protective instruments or measures.

ERPG3: This is the maximum airborne concentration that causes mortality in exposure with the substance.

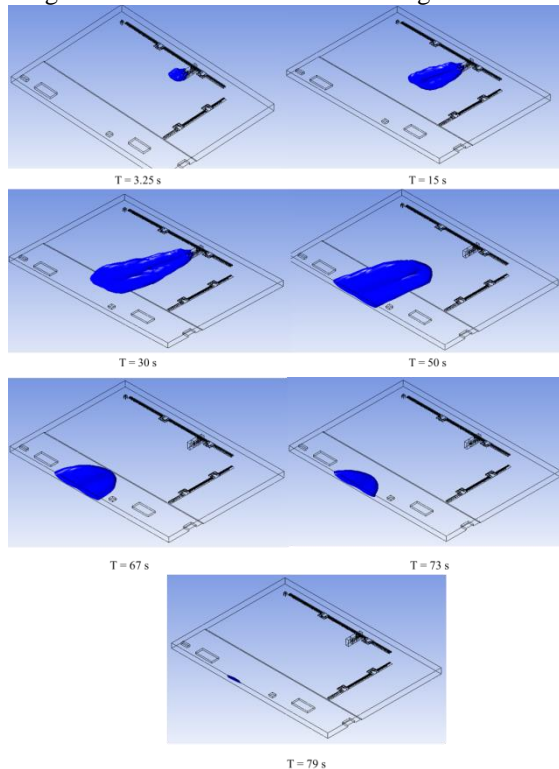
It is clearly shown in above diagrams that Rack structures in right side of port and administrative buildings in drought are not influenced of the ammonia release. Ammonia cloud developed moves in direction with wind, and exits from computational area about 85 seconds after ammonia release. Furthermore, according to concentration about 750 ppm, none of service buildings are influenced inside drought. Only control building next to port is



influenced of ammonia release. To examine emission effect, flow lines in different time intervals have been proposed. According to the type of ammonia emission, expected having uniform flow lines in flow field.

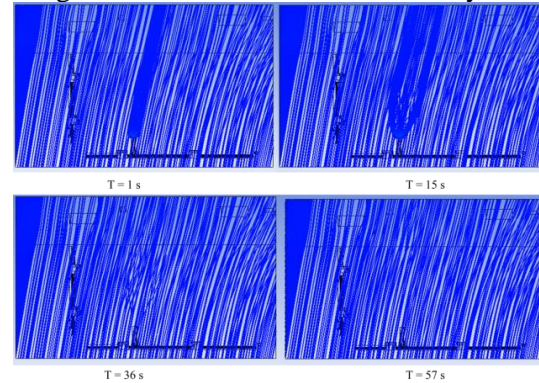


**Fig 12.** Constant concentration surfaces 150 ppm indicating ERPG2 for emission from loading arm



**Fig 13.** Constant concentration surfaces 750 ppm indicating ERPG3 for emission from loading arm

Vortex flow due to uniform ammonia concentration distribution in any moment has not to exist in computational area. These predictions can be observed as shown in Figs 14. Before ending emission from arm, high volume flow lines at arm area observed, and the reason for this lies in ammonia entry to computational area. Depleting ammonia entry to computational area and by the passage of time, flow moves to stationary flow.



**Fig 14.** Changes at flow lines in terms of time for emission from loading arm.

## CONCLUSION

Emission and dispersion of gas pollutants in industrial complexes is one of the hazardous factors with high financial and living loss for industrial complex and environment around it. As a result, forecast the occurrence scenarios and preparation for that is one of the most important measures in designing and using industrial complexes. The most important step to forecast measures during event and/or designing and optimizing industrial complexes, is the very modeling and simulating how pollutants emit in surrounding area.

This study aims to simulate the way gas pollutants emit in surrounding one of ports at southern Pars located at Asaluyeh. The scenario under study is sudden detachment of loading arm during ship loading. CFD method has been used to simulate ammonia dispersion at area. Results indicate that dispersion of pollutants at area is totally in three-dimensional mode. By the passage of time, dispersion of pollutant would be in direction with wind, and exits in direction with wind from the area. Regions under influence of pollutants and while the region is influenced followed by event, are examined.

Results of modeling indicated that Rack structures in right side of port and administrative buildings in drought would not be under influence of this emission. This goes on to 85 seconds later emission so far as ammonia cloud exits from

computational area. Furthermore, according to concentration about 750 ppm, none of service buildings are influenced inside drought. Only control building next to port is influenced of ammonia release. About the changes for flow lines in terms of time regarding type of emission based on what expected before modeling, vortex flows due to uniformity of ammonia concentration distribution at any moment have not to exist at computational area. Before ending emission from arm, more flow lines at arm area can be seen. Finally, due to lack of vortex flow and barriers, ammonia exits from computational area with wind speed. In general, it can say if this occurs, none of the areas around port would be influenced of lethal concentrations.

Finally, suggestions as follows to prevent events and reduce environmental and life consequences followed by events are presented:

#### SUGGESTIONS

- Periodic and regular technical supervisions, as well as non-destructive tests in maintenance programs in order to prevent corrosions at components of loading arm.

-Thorough technical inspection after completion of maintenance and replacement of components by maintenance unit, and before reboot the system to prevent process and operational failures during repairs and parts replacement.

-Appropriate technical inspect and use of redundancies to prevent improper system functioning, Structural defects, especially defects in components of the security system and its components.

-Embedding proper management and engineering facilities in terms of security in the area to prevent sabotage.

-Considering the engineering and management measures required in passive defense

-Timely notification via alarms and other communications equipment, to all affected areas to reduce casualties.

-Develop and follow an Emergency Response Plan (ERP)

-Holding emergency exercises for all individuals affected in areas ERPG3 and ERPG2

-Training plan at emergency occasions to all personnel in considered area and individuals outside the area that affected by dangerous and deadly concentrations of ammonia.

-Escape, evacuation Accumulation and discharge site, all personnel should be perpendicular to the direction of the wind.

-Holding relief and rescue training sessions for victims affected by ammonia.

-Training ammonia material safety data sheet and education, health and environmental hazards deriving from ammonia and the ways to deal with employees.

-Existence of proper personal protective equipment, especially gas masks and oxygen tanks to the required number at the areas influenced of ERPG2 and ERPG3.

-Regular inspections of warning systems as well as personal protective equipment specially filtered gas masks and oxygen cylinders regularly and periodically.

-Equipping all employees and operators of the adjoining dock and also personnel at emergency conditions to ammonia detectors

#### REFERENCES

1. Centers for Disease Control and Prevention-The Facts about Ammonia- Department of Health and Human Services, Atlanta (2004).
2. Y. Tominaga, T. Stathopoulos, *Atm. Environ.* **47**, 8091 (2013).
3. S.B. Sutton, H. Brandt, B.R. White, *Boundary-Layer Meteorol.*, **35**, 125 (1986).
4. G.A. Perdikaris, F.J. Mayinger, *Loss Prevent. Process Ind.*, **2**, 10 (1994).
5. R.C. Hall, Proc. 1998 Hazards XIV, **12** (1998).
6. M.A. McBride, M. A., Reeves, A. B., Vanderheyden, M. D., Lea, C. J., & Zhou, X. X. *Process Safety Environ. Prot.*, **5** (2001).
7. S. Sklavounos, F. Rigas, *J. Hazard. Mater.*, **20**, 4 (2004).
8. F. Gavelli, E. Bullister, H. Kytomaa, *J. Hazard. Mater.*, **10**, 5, (2008).
9. Yu Hong-xi et al., *J. China Univ. Petrol.*, **40**, 3 (2008).
10. A. Mazoldi, T. Hill, J.J. Colls, *Atm. Environ.*, **42**, 8046 (2008).
11. E. Kashi, F. Shahraki, D. Rashtchian, Behzadmehr, Iran. *J. Chem. Eng.*, **6**, 26 (2009).
12. B.R. Cormier, Qi R., Yun G., Zhang Y., M.J. Sam Mannan, *Loss Prev. Proc. Ind.*, **30**, 3 (2009).
13. Zhang C.N., Ning P., Ma C.X., *J. Wuhan Univ. Technol.*, **15**, (2009).
14. F. Gavelli, M.K. Chernovsky, E. Bullister, H.K. Kytomaa, *J. Hazard. Mater.*, **25**, 4 (2010).
15. M. Siddiqui, S. Jayanti, T. Swaminathan, *J. Hazard. Mater.*, **32**, 7 (2012).
16. H.K. Versteeg, W. Malalasekera, *An Introduction in Computational Fluid Dynamics*, Prentice Hall, 2nd Edition, 2007, p. 17.
17. I.G. Currie, *Fundamental Mechanics of Fluids*. Marcel Dekker Inc., 1993.
18. V. Yakhot, S.A. Orszag, *J. Sci. Comp.*, **7**, 4 (1986).
19. M.E. Davies, S. Singh, *J. Hazard. Mater.*, **10**, 5 (1985).
20. S.R. Hanna, In: *Tracking and Predicting the Atmospheric Dispersion of Hazardous Material Releases: Implication of Homeland Security*, The National Academies Press. N.Y., 2003, pp. 66-69.

21. Harvard School of Public Health, Boston. [http://books.nap.edu/openbook.php?record\\_id%2F410716&page%2F469](http://books.nap.edu/openbook.php?record_id%2F410716&page%2F469).
22. D.C. Thoman, K.R. O'Kula, J.C. Laul, M.W. Davis, K.D. Knecht, *J. Chem. Health Safety*, **13**, 4 (2006).
23. D.O.E., U.S., Software Quality Assurance Improvement Plan: ALOHA Gap Analysis. Office of Environment, Safety and Health; U.S. Department of Energy, Washington. EH-4.2.1.3 (2004).
24. S.R. Hanna, O.R. Hansen, S. Dharmavaram, *Atm. Environ.*, **38**, 4675 (2004).
25. A. Venkatram, A. Tripathi, Proc. Fourth Workshop on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. Oostende, Belgium, **14**, (1996).