

## SIIC065

### DYNAMIC RISK MODELLING OF A CHEMICAL REACTOR USING ASPEN PLUS

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#### **Abstract:**

Risk assessment is an important step in predicting possible threats of hazards. The objectives of this research project are to identify potential risks that could possibly occur to a chemical reactor in a dynamic environment by using Fault Tree Analysis (FTA), and to simulate and evaluate the risks of a chemical reactor in a dynamic environment by using Aspen Plus and Bayesian Network. In a dynamic situation, a conventional risk assessment is lacking in providing the information needed. Aspen Plus is one of the most leading software used in the industry as it could be used to comprehend the condition of the reactor in a faulty condition. Sensitivity analysis is simulated in dynamic condition to observe the behavior of the methanol. The highest mole flow of methanol is produced when the model is deviated to 262 bars. Threats and severity of any faulty conditions such as leakage of reactor or thermal radiation from jet fire could be predicted by using Areal Location of Hazardous Atmosphere (ALOHA). From the leakage of the reactor, a small but dense flame pocket of concentration greater than 43080 ppm is detected. A threat of potentially lethal within 60 seconds is predicted as the thermal radiation from jet fire is simulated. From the point, the area of coverage for the threat is 1.38 yards off centerline and 1.72 yards downwind. A second-degree pain is possible at off centerline of 1.21 yards and 11.2 yards downwind. Fault tree analysis could be constructed based on the model simulations as the faults that caused the risk has been determined. A Bayesian Network could also be constructed as the threats from the risk also has been determined.

#### **Keywords:**

*Dynamic risk modelling, Aspen Plus, Bayesian Network, Areal Location of Hazardous Atmosphere (ALOHA), Fault Tree Analysis (FTA).*

#### **Objectives:**

- To identify potential risks that could possibly occur to a chemical reactor by using Fault Tree Analysis (FTA), and
- To simulate and evaluate the risks of a chemical reactor in a dynamic environment by using Aspen Plus, ALOHA and Bayesian Network.

**Methodology:**

**Sensitivity Analysis by Aspen Plus**

- Sensitivity analysis is modelled by using simulation from a previous study supervised by the same supervisor. Pressure of the reactor is manipulated to observe the mole flow and mass fraction of methanol at the outlet stream of the reactor.



**Risk Modelling**

- Based on the highest mole flow and mass fraction of the methanol at the manipulated pressure, risk could be modelled by simulating the environment of selected area, which is Khark Petrochemical Complex, Iran in ALOHA software. The environment and geographical structure of the site is simulated in the software. Chemical information and reactor information are obtained from the simulation used for sensitivity analysis. Risks are modelled based on two leakage apertures.



**Fault Tree Analysis**

- Hazards are identified based on the previous simulations.

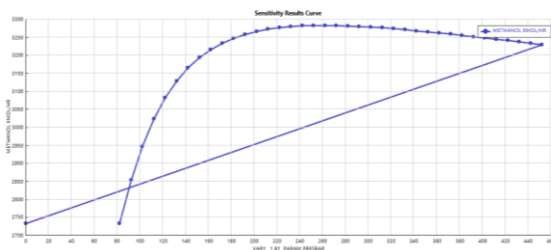


**Bayesian Network**

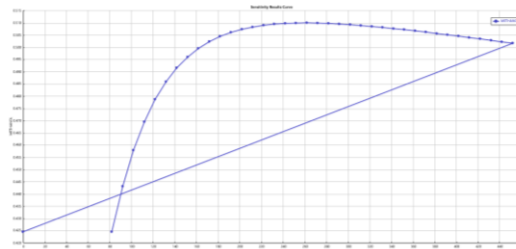
- Occurrence probability of the risk is modelled by using Bayesian Network, which is constructed by using GeNie Modeler (GeNie Academic 2.5).

**Results:**

***Sensitivity Result Curve of Pressure vs. Methanol Mole-Flow***



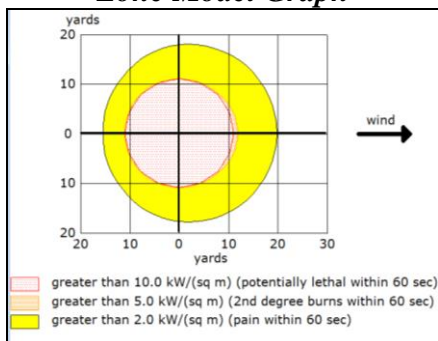
***Sensitivity Analysis Curve of Pressure vs. Methanol Mass Fraction***



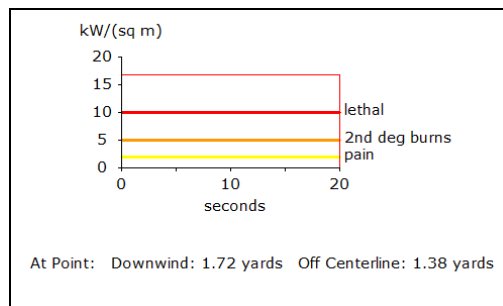
***Thermal Radiation from Jet Fire Threat***

***Lethal Time vs. Area of Threat Zone of Thermal***

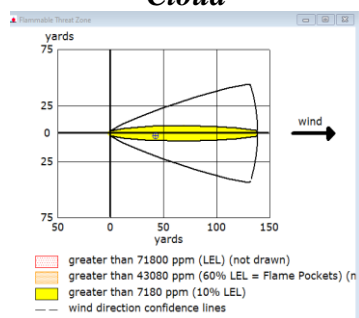
**Zone Model Graph**



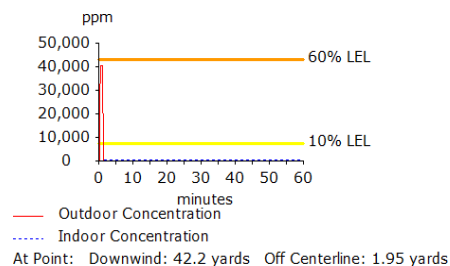
**Radiation from Jet Fire**



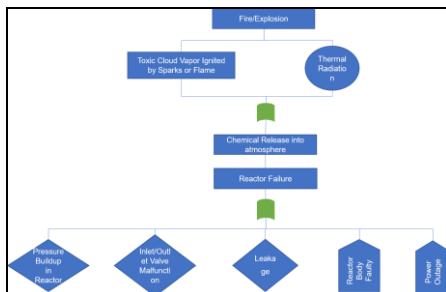
**Flammable Threat Zone Graph of Vapor Cloud**



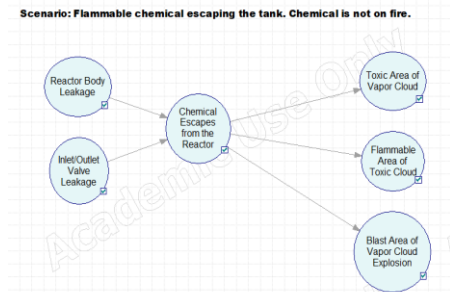
**Time vs Concentration Graph of Flammable Threat Zone of Vapor Cloud**



**Fault Tree Diagram**



**Bayesian Network**



**Conclusion:**

In conclusion, the objectives of the research project are achieved. Potential risks that could possibly occur to a chemical reactor is able to be identified by using Fault Tree Analysis (FTA). Simulation and evaluation of the risks of a chemical reactor in a dynamic environment by using Aspen Plus, ALOHA and Bayesian Network are able to be simulated without any error. By using Aspen Plus, sensitivity analysis of reactor could be conducted to predict the behavior of the reactor at a dynamic environment in terms of pressure. The simulation used a plug flow reactor at pressure of 82 bar. Deviation of pressure with an increment of 10 bar was conducted and it is identified at 262 bar, the reactor produced methanol at mole fraction of 0.51. From the data obtained, environment of Kharg Island, Iran is simulated by using ALOHA to identify and evaluate the risk of the reactor in dynamic environment thus improving the existing risk assessment for a safer future of industrial processes and environmental.