


**Air pollutants concentration changes and exposure risk levels in the most important petrochemical complexes zone, Iran**

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## Importance

- Petrochemical industries are the major emission sources of VOCs in the atmosphere.
- It is clear that some of the VOCs have the potential impact on human health and are toxic.
- These pollutants can accumulate in the organisms.
- A lot of petrochemical complexes release high amounts of air pollutants in the atmosphere around the PET Zone, continuously.



## Main Goals

- Determination of Benzene, Hexane, Toluene, Xylene, Phenol, Ethyl Benzene, Ethylene glycol, Formaldehyde, Acetaldehyde concentration in the greatest petrochemical complex zone in Iran (PET Zone)
- Determination of Toluene diisocyanate concentration in PET Zone
- Determination of Particulate Matter concentration in PET Zone
- Determination of Heavy Metals and Hg concentration in PET Zone
- Air quality assessment based on results comparison with standard levels
- Exposure risk assessment with volatile organic components in this area



## Properties of studied pollutants and their effects

• Benzene	• Ethylene glycol
• Toluene	• Formaldehyde
• Xylene	• Acetaldehyde
• Ethyl Benzene	• TDI and MDI
• Hexane	• Butadiene
• Phenol	• PM
• Trace elements	• Hg

## (Benzene)

• Structural formula: $C_6H_6$	• Odor:
• Molecular weight: 78.11	Lower: 0.84 ppm
• Vapor pressure: 75 mm Hg at 20°C	Upper: 53 ppm
• Water solubility: 1750 mg/L at 25°C	• Benzene is rapidly distributed throughout the body after exposure by all routes, and accumulation in fatty tissues is observed
• Conversion factor: 1 ppm = 3.24 mg/m <sup>3</sup> at 20°C; 1 mg/m <sup>3</sup> = 0.31 ppm;	• PEL (permissible exposure limit) TWA = 1 ppm (OSHA, 1987)
• Boiling point: 80.1°C at 760 mm Hg	• TLV (threshold limit value) TWA = 10 ppm (ACGIH, 1996)
• Taste threshold: 0.5 to 4.5 mg/L	

## (Toluene)

• Structural formula: $C_6H_5CH_3$	• Chronic inhalation exposure of humans to toluene causes irritation of the upper respiratory tract and eyes, sore throat, dizziness, headache, and difficulty with sleep
• Molecular weight: 92.14	• Toluene is absorbed into the blood is distributed throughout the body
• Density: 0.867 g/mL	• PEL (permissible exposure limit) TWA = 200 ppm (754 mg/m <sup>3</sup> )
• Vapor pressure: 28.4 mm Hg at 25 oC	• TLV (threshold limit value) TWA = 50 ppm (189 mg/m <sup>3</sup> ) (ACGIH, 2000)
• Water solubility: 0.59 mg/mL at 25 oC	
• Conversion factor: 1 ppm = 3.77 mg/m <sup>3</sup> , 1 mg/m <sup>3</sup> = 0.265 ppm (25 oC, 760 mmHg)	

### (Xylene)

- Structural formula: C<sub>8</sub>H<sub>10</sub>
- Molecular weight: 106.17
- Vapor pressure: 6–16 mmHg mixture at 20°C
- Density: 0.864 g/cm<sup>3</sup> mixture
- Solubility in water: 130 mg/L mixture
- Conversion factor:  
1 ppm = 4.34 mg/m<sup>3</sup>; 1 mg/m<sup>3</sup> = 0.23 ppm
- Odor threshold in air:  
1.0 ppm mixture
- Xylenes are rapidly absorbed following both inhalation and oral exposure.
- Following absorption, considerable metabolism occurs, with the liver being the primary site of metabolism. Xylenes are distributed throughout the body, but show the greatest affinity for lipid-rich tissues such as the brain.
- Elimination is rapid and occurs primarily in the urine, with the predominant form being the glycine conjugate of methylbenzoic acid (methylhippuric acid).
- PEL (permissible exposure limit) TWA = 100 ppm (OSHA, 2003)



### (Ethyl benzene)

- Structural Formula: C<sub>8</sub>H<sub>10</sub>
- Density @ 20 °C (g/mL): 0.867
- Boiling Point (°C): 136.2
- Odor threshold around: 0.5 ppm.
- Possible effects: nearing 100 ppm
- Irritation for 8 hour per day exposures at 100 ppm. Eye irritation at 200 ppm.
- Tolerance can be built at 1000 ppm levels, though first exposure very irritating to eyes.
- Immediate eye irritation at 2000 ppm. 5000 ppm intolerable irritation of eyes, nose and throat, chest constriction, eye irritation, dizziness, effects on blood, liver, and kidneys
- Cancer ranking: EPA does not classify ethyl benzene as a carcinogen
- PEL (permissible exposure limit) TWA = 100 ppm (OSHA, 2003)

### (Hexane)

- Structural formula: C<sub>6</sub>H<sub>14</sub>
- Molecular weight: 86.18
- Vapor pressure: 151.3 mm Hg at 20°C
- Water solubility: 1750 mg/L at 25°C
- Boiling point: 68.7°C at 760 mm Hg
- Low level (<50 ppm): Nerve cell death over lifetime exposures.
- Medium level (50 - 500): Evidence of nerve cell death over long term (lifetime) exposures. As concentration increases, less time necessary for nerve cell death to occur. Odor recognition around 130 ppm.
- High level (500 - 1000 ppm): Eye and upper respiratory track irritation. Nerve cell death after a few months exposure.
- Very High level (>1000 ppm): For short time frames (10 minutes) very little effect at 2000 ppm. 5000 ppm for 10 minutes causes dizziness. Some giddiness, nausea, headache, eye and throat irritation. Depression, respiratory arrest, and nerve cell death.
- Cancer ranking: EPA has not classified hexane as a human carcinogen.
- TWA = 50 ppm (NIOSH, 2003)
- TLV (threshold limit value) TWA = 50 ppm (ACGIH, 2003)

### (Phenol)

- Structural formula: C<sub>6</sub>H<sub>6</sub>O
- Molecular weight: 94.12
- Vapor pressure: 0.3513 mm Hg at 20°C
- Water solubility: 87 mg/L at 25°C
- Conversion factor:  
1 ppm (v/v) = mg/m<sup>3</sup> x 0.260  
1 mg/m<sup>3</sup> = ppm (v/v) x 3.85
- Boiling point: 181.8°C at 760 mm Hg
- Odor threshold:  
0.047 ppm (0.18 mg/m<sup>3</sup>) - 100% response  
0.006 ppm (0.02 mg/m<sup>3</sup>) - sensitive
- Phenol is absorbed by the inhalation, and oral routes. phenol is widely distributed in the body, although the levels in the lung, liver, and kidney are often reported as being higher than in other tissues.
- Elimination from the body is rapid, primarily as sulfate and glucuronide conjugates in the urine.
- Phenol does not appear to accumulate significantly in the body.
- PEL (permissible exposure limit) TWA = 5 ppm (OSHA, 1987)

### (Acetaldehyde)

- Structural formula: C<sub>2</sub>H<sub>4</sub>O
- Conversion factor:  
1 ppm = 1.80 mg/m<sup>3</sup>
- Boiling point: 20.8 °C at 760 mm Hg
- Eye contact: Immediately flush the eye with water. Continue for at least ten minutes and call for immediate medical help, since acetaldehyde may burn the eyes.
- Skin contact: Wash off with plenty of water. Remove any contaminated clothing. If the skin reddens or appears damaged, call for medical aid.
- PEL (permissible exposure limit) TWA = 0.75 ppm (OSHA, 1987)
- TLV (threshold limit value) TWA = 0.1 ppm (NIOSH, 2003)

### (Formaldehyde)

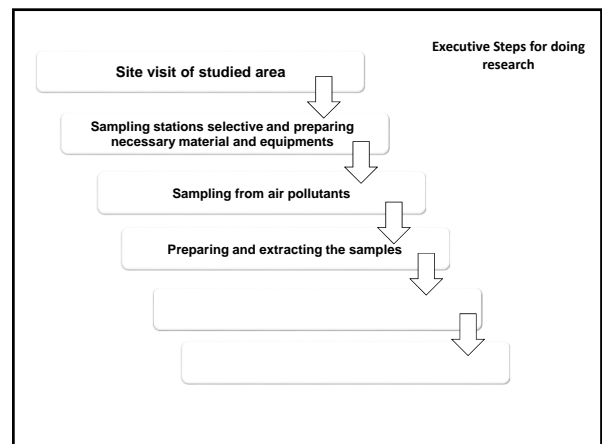
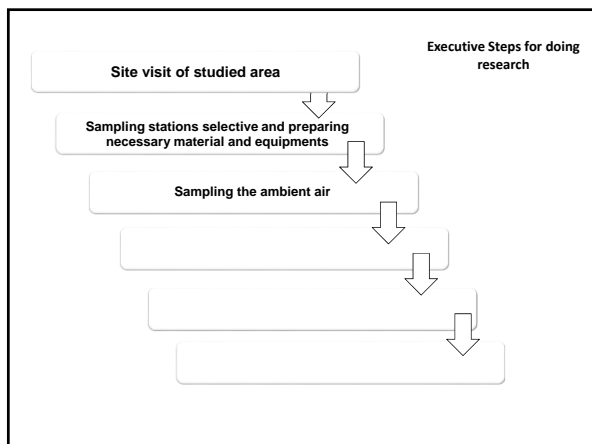
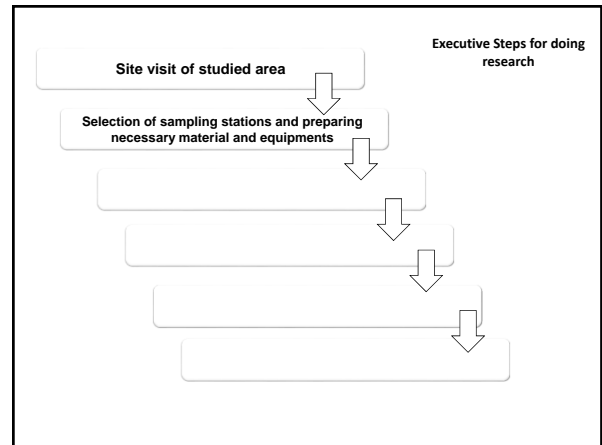
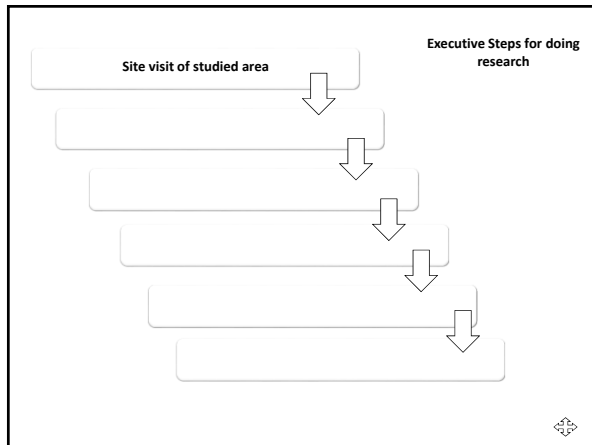
- Structural formula: H<sub>2</sub>C=O
- Vapor pressure: 55 mm Hg at 20°C
- Conversion factor:  
1 ppm = 1.23 mg/m<sup>3</sup> at 20°C;
- Boiling point: 96°C at 760 mm Hg
- TLV (threshold limit value) TWA = 0.3 ppm (ACGIH, 1996)
- Causes burns. Very toxic by inhalation, ingestion and through skin absorption. Readily absorbed through skin. Probable human carcinogen. Mutagen. May cause damage to kidneys, allergic reactions, sensitisation, heritable genetic damage. Lachrymator at levels from less than 20 ppm upwards. Very destructive of mucous membranes and upper respiratory tract, eyes and skin.
- PEL (permissible exposure limit) TWA = 0.75 ppm (OSHA, 1987)

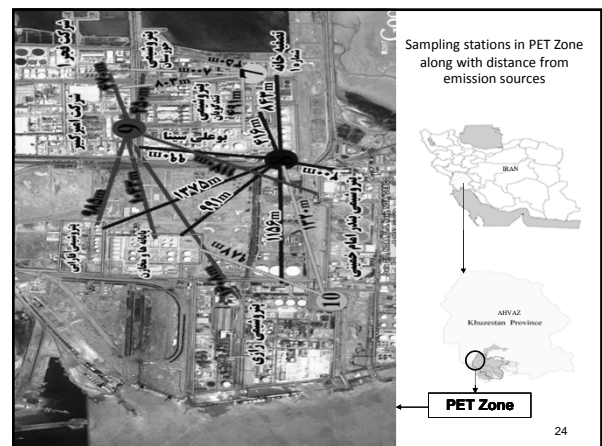
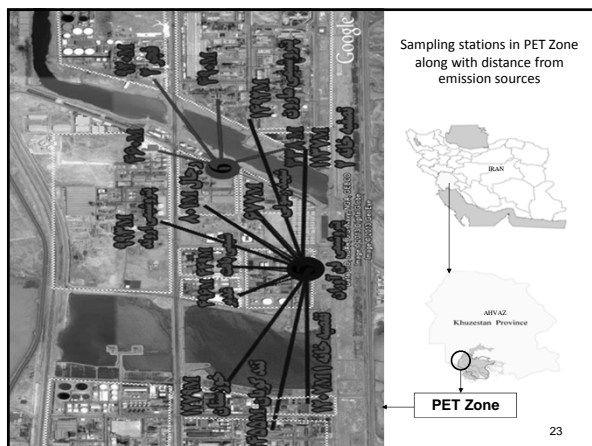
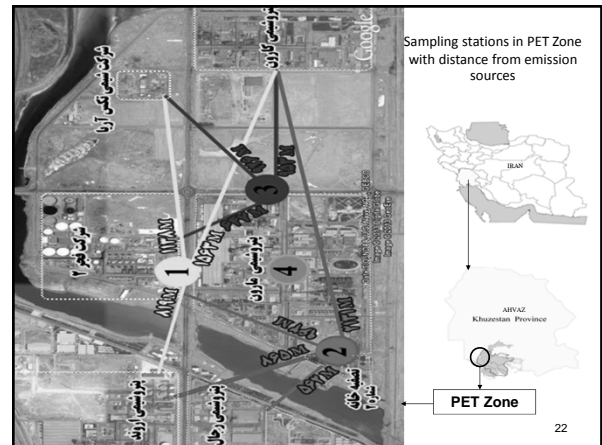
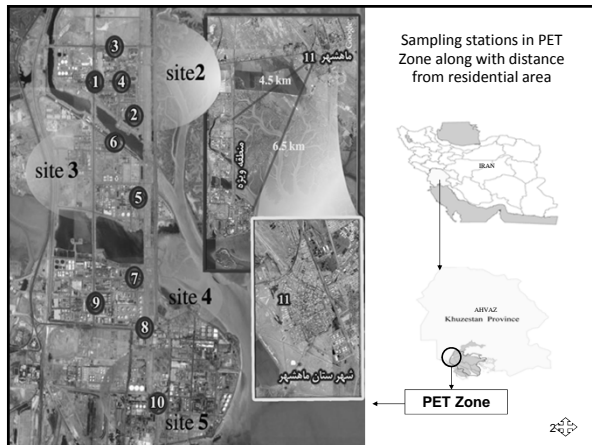
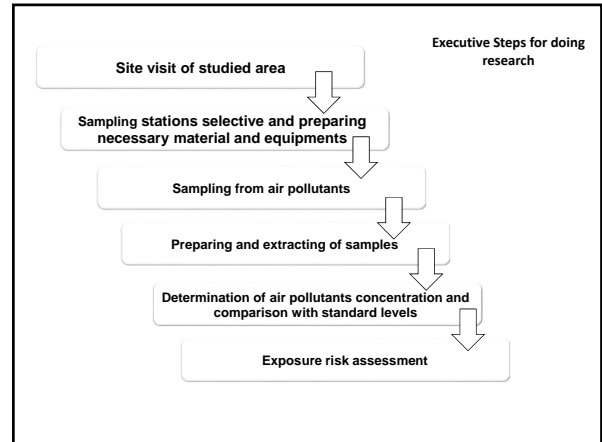
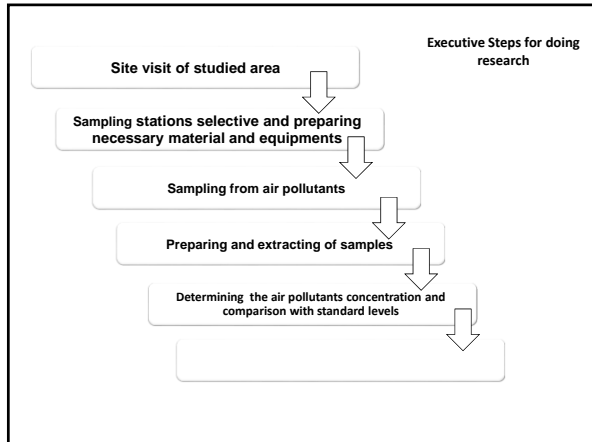
**(TDI)**

- Structural formula: C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>
- Molecular weight: 174.16 g/mol
- Vapor pressure: 0.008 mm Hg at 20°C
- Conversion factor:  
1 ppm = 7.1 mg/m<sup>3</sup> at 20°C;
- Boiling point: 251°C at 760 mm Hg
- REL (Reference exposure limit) = 0.07 ppb
- Low level (<0.002 ppm; <0.014 mg/m<sup>3</sup>) exposures in occupational settings can lead to chronic loss of lung function, including bronchitis or asthma. A higher level (0.002 - 0.02 ppm) of exposure may lead to immune response from repeated exposures. 10 to 20 minute exposures at these concentrations may lead to delayed asthmatic responses in people sensitized to this chemical. Decreased lung function can occur after longer exposures. Even higher exposures, from spills or fires, may lead to neurological problems.
- Cancer ranking: the International Agency for Research on Cancer (IARC) has classified 2,4-toluene diisocyanate as a Group 2B, possible human carcinogen for a variety of tumors.

**Material and Methods**

- Executive Steps for doing this research
- Determining the sampling stations
- Sampling equipments and necessary materials
- Sampling and analysis methods
- Calculations and exposure risk assessment





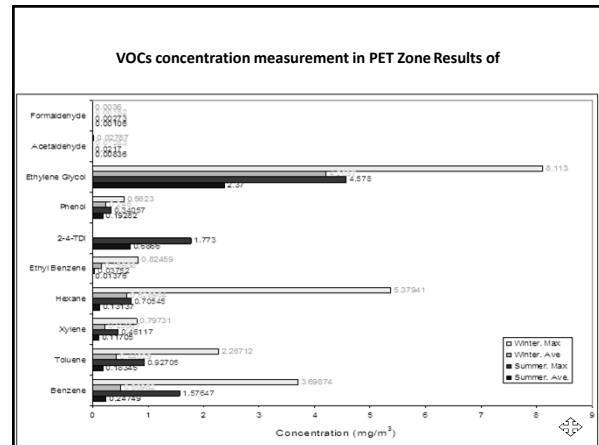
### Studied parameters

Chemical formula	Pollutant	No.
C <sub>6</sub> H <sub>6</sub>	Benzene	1
C <sub>7</sub> H <sub>8</sub>	Toluene	2
C <sub>8</sub> H <sub>10</sub>	Xylene	3
C <sub>6</sub> H <sub>14</sub>	Hexane	4
C <sub>2</sub> H <sub>4</sub> O	Ethylene glycol	5
CH <sub>2</sub> O	Formaldehyde	7
C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde	8
C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> CH <sub>2</sub> C <sub>2</sub> H <sub>4</sub> (NCO) <sub>2</sub>	2-4-TDI	9
C <sub>6</sub> H <sub>5</sub> OH	Phenol	10
H <sub>2</sub> C=CHHC=CH <sub>2</sub>	1-3-Butadien	11
-	Trace elements	12
Total suspended particle	TSP	13

### Used sorbents and filters in sampling process

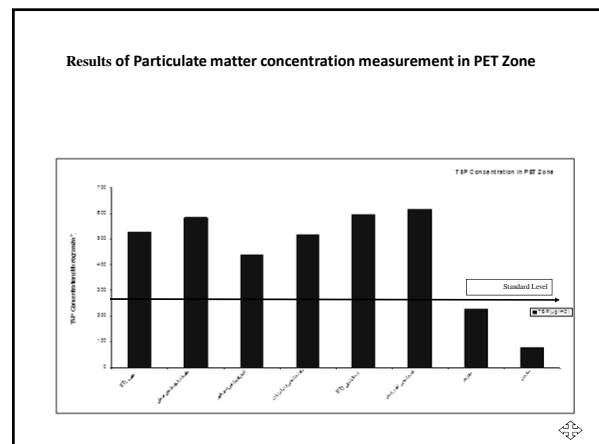
Sampler identification Code	Sampler Type	Pollutant	No.
226-01	Sorbent solid	Benzene	1
226-01	Sorbent solid	Toluene	2
226-01	Sorbent solid	Xylene	3
226-01	Sorbent solid	Hexane	4
226-35-03, 226-57	Sorbent solid	Ethylene glycol	5
226-119	Sorbent solid	Formaldehyde	6
226-119	Sorbent solid	Acetaldehyde	7
225-9002	Coated filter	2-4-TDI	8
226-95, 225-5	Sorbent solid	Phenol	9
226-09	Sorbent solid	1-3-Butadien	10
-	Filter and on-line system	PM	11

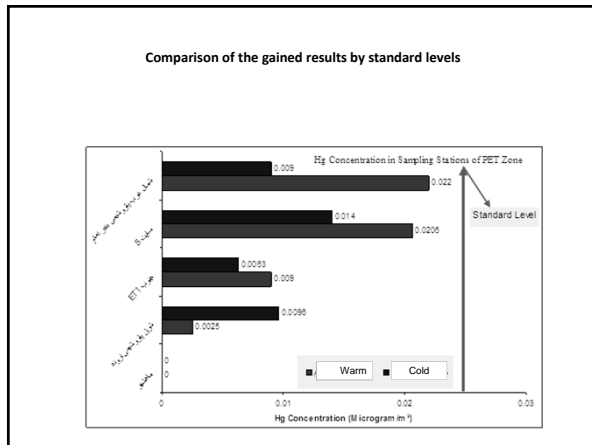
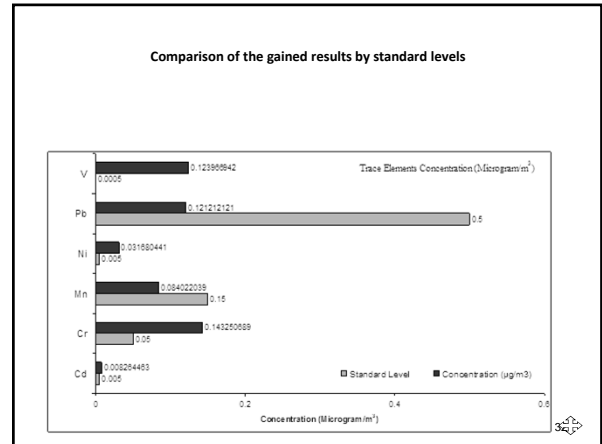
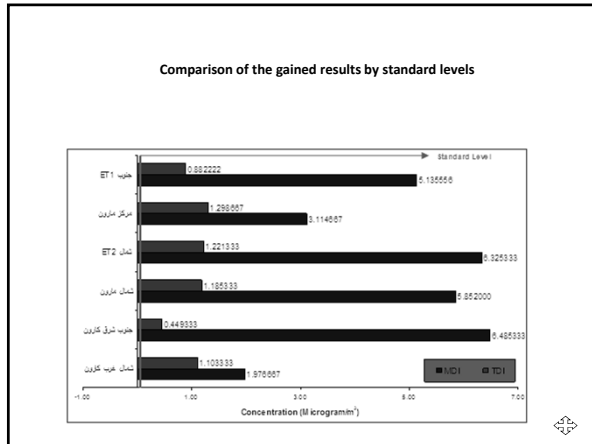
## Results



### Comparison of the gained results by standard levels (summer 2010)

TDI	Phenol	Ethylbenzene	Xylene	Toluene	Benzene	مقدار استاندارد
N.D	0.28341	0.00213	0.00192	0.02167	0.00477	1
1.773	0.34057	0.00235	0.00235	0.02568	0.00588	2
0.666	0.33635	0.02035	0.26705	0.03569	0.05176	3
0.226	0.16875	0.01529	0.04117	0.08253	0.07294	4
0.08	0.094472	0.03759	0.15348	0.34118	0.29411	5
-	0.13659	0.02213	0.46117	0.92705	1.57647	6
-	0.21045	0.01142	0.085314	0.31724	0.23713	7
-	0.08054	0.00505	0.00858	0.00894	0.01176	8
-	0.10421	0.00495	0.01117	0.00423	0.01764	9
-	0.20447	0.00235	0.04117	0.03176	0.05058	10
-	0.16826	0.00729	0.10305	0.05929	0.04480	11
-	0.18864	0.03423	0.22811	0.34638	0.60214	12
0.6866	0.19282	0.01376	0.11705	0.18345	0.24749	Mean
0.00007	0.2	1	0.1	0.3	0.03	Standard





Exposure risk assessment of air pollutants in the studied area

Exposure risk of benzene in the PET zone

Time/Range	Concentration	RFC (mg/m³)	Current Risk	Allowable risk
Summer, Min	0.00477	0.03	2.69186E-06	1.69299E-05
Summer, Max	1.57647	0.03	0.000889652	1.69299E-05
Summer, Average	0.24749	0.03	0.000139666	1.69299E-05
Winter, Min	0.00723	0.03	3.84011E-06	1.59341E-05
Winter, Max	3.69874	0.03	0.001964532	1.59341E-05
Winter, Average	0.509823333	0.03	0.000270785	1.59341E-05
Total Average	0.378656667	0.03	0.000206628	1.63706E-05

Exposure risk of Ethyle-benzene in the PET zone

Time/Range	Concentration	RFC (mg/m³)	Current Risk	Allowable risk
Summer, Min	0.00213	1	1.03623E-07	4.86493E-05
Summer, Max	0.03752	1	1.82532E-06	4.86493E-05
Summer, Average	0.013755	1	6.69171E-07	4.86493E-05
Winter, Min	0.00236	1	1.08059E-07	4.57875E-05
Winter, Max	0.82459	1	3.7756E-05	4.57875E-05
Winter, Average	0.159383333	1	7.29777E-06	4.57875E-05
Total Average	0.086569167	1	4.07239E-06	4.7042E-05

Exposure risk of TDI in the PET zone

Time/Range	Concentration	RFC (mg/m <sup>3</sup> )	Current Risk	Allowable risk
Near Karun Petrochemical	1.22	0.00007	2.61149E-07	1.4984E-11
Near Marun Petrochemical	0.15333	0.00007	3.28213E-08	1.4984E-11
Summer, Average	0.68666	0.00007	1.46984E-07	1.4984E-11



Exposure risk of phenol in the PET zone

Time/Range	Concentration	RFC (mg/m <sup>3</sup> )	Current Risk	Allowable risk
Summer, Min	0.080548594	0.2	3.1349E-05	7.78388E-05
Summer, Max	0.340573656	0.2	0.000132549	7.78388E-05
Summer, Average	0.192822442	0.2	7.50454E-05	7.78388E-05
Winter, Min	0.062795879	0.2	2.30022E-05	7.32601E-05
Winter, Max	0.562308549	0.2	0.000205974	7.32601E-05
Winter, Average	0.245000511	0.2	8.97438E-05	7.32601E-05
Total Average	0.218911477	0.2	8.23843E-05	7.52672E-05



Exposure risk of Acetaldehyde in the PET zone

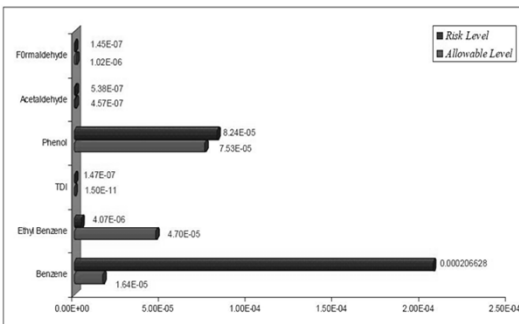
Time/Range	Concentration	RFC (mg/m <sup>3</sup> )	Current Risk	Allowable risk
Summer, Min	0.0006	0.009	3.15247E-08	4.72871E-07
Summer, Max	0.021733333	0.009	1.1419E-06	4.72871E-07
Summer, Average	0.008361111	0.009	4.39303E-07	4.72871E-07
Winter, Min	0.000866667	0.009	4.28571E-08	4.45055E-07
Winter, Max	0.027866667	0.009	1.37802E-06	4.45055E-07
Winter, Average	0.012827778	0.009	6.34341E-07	4.45055E-07
Total Average	0.010594444	0.009	5.38255E-07	4.57248E-07



Exposure risk of Formaldehyde in the PET zone

Time/Range	Concentration	RFC (mg/m <sup>3</sup> )	Current Risk	Allowable risk
Summer, Min	0	0.009	0	1.05082E-06
Summer, Max	0.002733333	0.009	3.19139E-07	1.05082E-06
Summer, Average	0.001059444	0.009	1.23699E-07	1.05082E-06
Winter, Min	0	0.009	0	9.89011E-07
Winter, Max	0.0036	0.009	3.95604E-07	9.89011E-07
Winter, Average	0.001517222	0.009	1.66728E-07	9.89011E-07
Total Average	0.001288333	0.009	1.45454E-07	1.01611E-06

Comparison of studied air pollutants exposure risk by permissible risk levels



Conclusion

It is very important that industrial areas, specially similar to PET - Zone should have comprehensive plan for air pollution control. This plan must include :

- Identification of all emission sources such as stacks, storage tanks, valves, wastewater ponds and etc.
- Measurement of all VOCs and other pollutants such as trace elements and preparing a complete data bank.
- Application of air pollution dispersion and emission modeling in these areas
- Estimating vapor emission from storage tanks and flares.
- Calculation the emission factors for all pollutants from all sources and also determination their emission share.
- Finally, preparing the emission reduction methods for all sources according to each pollutant.



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Thank you for your attention

