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Modeling of the BTX Species Based on an Emission Inventory of Sources at the Map Ta Phut Industrial Estate in Thailand

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ABSTRACT: Air emissions from the Map Ta Phut petrochemical complex in southeastern Thailand were studied. One focus of the research is the development of an emission inventory of the volatile organic compounds, benzene, toluene, and xylene (BTX). Emission sources were identified and the loading from all mobile and stationary sources were compiled. Based on this data set, the Industrial Source Complex Short-Term version 3 (ISCST-3) was used to predict the contributions of the BTX species, which then were compared with the field measurements. The methodology of the emission inventory is described and evaluated with the shortcomings and areas of uncertainty. The relative importance of point, line and area sources and the influence of the local meteorology on the timing and place of concentration impacts are discussed. The coincidences and differences observed highlight the relative importance of source type and location, and of fugitive emissions and episode events. In particular, this research highlights the importance of area emissions from the petrochemical and petroleum industries, such as the oil refineries and tank farms, and identifies them as potential major contributors to the ambient BTX concentrations.

KEYWORDS: BTX, Emission Inventory, ISCST-3, Source Modeling, Thailand.

INTRODUCTION

The investigation of volatile organic compounds (VOCs) emissions in the atmosphere is of great interest. This interest is because of the great variety of VOCs existing in the atmosphere in variable concentrations, which can have serious implications for the environment and public health. Organic compounds play a variety of roles in many air environmental problems, including formation of ground-level photochemical ozone, enhancement of the global greenhouse effect and depletion of stratospheric ozone. Additionally, some species can cause serious health effects through toxic, carcinogenic, mutagenic, or neurotoxic actions. Benzene is recognized today as one of the more hazardous VOC species.

The Map Ta Phut industrial estate in southeastern Thailand was established in the early 1990's. It serves as the upstream industrial estate for many petrochemical-related industries. The complexity and integration of the estate operations have caused various air pollution problems, including odor and health-related ones, from the various air emissions. In June 1997, 120 students at a secondary school, located to the northeast of the estate, were affected by chemical vapors released from the factories in the estate. The students reported having dizziness, headaches, nasal inflammation, throat soreness and tiredness[1]. Furthermore, offensive odors from the factories in the estate are still recorded regularly with mitigation being handled on a case by case base. These types of reports have heightened public concerns about gaseous emissions from the petrochemical industry in general. Recently, there have been protests against a gas pipeline project in the south of Thailand due to concern about potential emissions[2].

There are some preliminary studies of VOC in the general area and from the emissions at Map Ta Phut. Two studies were conducted to detect VOC species and assess ambient concentration levels. Fourteen species were detected, and benzene, toluene and xylene were reported in range of 1.4-3.5, 0-22 and 0.8-20 $\mu g\ m^{-3}$, respectively[3,4]. Data from these studies were preliminary and very limited and no long term or variable condition

assessments were made. In 1999, the Thailand Environment Institute (TEI) was awarded a contract from NEDO to study the sources of air pollution, mainly for air particulate matter and gaseous SO_x and NO_x species. TEI collected data via a factory survey and reported that 15 factories in the Map Ta Phut area emitted VOCs from fuel combustion, leakage from manufacturing processes, storage, and incineration[5]. In addition, the Industrial Estate Authority of Thailand (IEAT) in cooperation with Department of Industrial Works (DIW), Pollution Control Department (PCD) and the Office of Environmental Policy and Planning (OEPP) are conducting a study on the carrying capacity of the area for particulate SO_x and NO_x, but not addressing VOCs. Thus, there is a need to carry out further research concerned with the impact of VOC air emissions from the Map Ta Phut petrochemical complex on surrounding areas.

This paper presents the development of an emission inventory of the volatile organic compounds, benzene, toluene and xylene (BTX) and application of the Industrial Source Complex Short-Term (ISCST-3) air model to assess the impacts of the inventory on ambient air quality in and around the complex under varying meteorological conditions. The applied methodologies and the resulting database are of on-going values in developing effective measures to manage air pollution problems and provide a basic approach for dealing with VOCs emissions in other areas as well.

Methodology

The Map Ta Phut Industrial Estate is situated in the Rayong Province about 200 kilometers southeast of Bangkok, at location 12° 30' N and 101° 35' E. It covers an area of about 6,000 Rai (960 hectare) and has approximately 10,000 workers. The estate was established under the Eastern Seaboard Program during the Fifth National Economic and Social Development Plan when Thailand proposed to make use of natural gas from the Gulf of Thailand. Gas pipes were constructed extending from the Gulf of Thailand to Tambon Map Ta Phut for hydrocarbon separation before the actual use. At that time, the Thai Government foresaw the geographic importance of Tambon Map Ta Phut in serving heavy industrial factories, which use natural gas as a primary raw material. The Map Ta Phut Industrial Estate was thus established to serve these needs. Currently, there are 52 factories, of which 32 factories are petroleum-related industry[6]. There are also two other industrial estates, Padaeng and the Eastern Industrial Estate, located on the western border of the estate, which make for a total of 86 factories in the same sub-regional air basin. There is a deep-sea port within the estate and a major road, Sukhumvit Road, passes close to the estate. This is the main road to the eastern part of Thailand, a very popular tourist area. The estate is also surrounded by existing dwellings.

The weather in Map Ta Phut is very similar to other coastal regions in the country. There are basically three seasons: the hot season, the rainy season and the cool or dry season. Average temperatures are 24-37 °C. The highest mean level of rainfall is approximately 267 mm per month during September. The relative humidity is around 60-95 %. The Map Ta Phut area is influenced by the sea wind, which sweeps from the southwest to the northeast with a wind speed typically below 6 m s^{-1}. The location and layout area is shown in Fig. 1.

Compilation of an Emission Inventory

The methodologies for compiling hazardous air pollutants have been reported in various studies[7, 8, 9]. Typically, emission data are based on some combination of measurement, survey and calculation. The main classes of the emission data were summarized by Lagoudi[9], as the following categories:

Class M: Emission data that are based on measurements using standardized or accepted methods; often additional calculations are needed to convert the results of measurements into annual emission data.

Class C: Emission data that are based on calculations using nationally or internationally accepted estimation methods and emission factors, which are representative for the industrial sectors.

Class E: Emission data that are based on non-standardized estimations derived from best assumptions or expert guesses.

In this research, a combination of both top-down and bottom-up approaches[8,10] has been used. Primarily, the bottom-up approach was preferred and generally used. The top-down approach was used to determine some potential sources of BTX, including estimating the projected mobile loading in the area. The methodology included identification the of BTX sources as point, area and line sources, through site visits to the factories. Detailed information about all operational units in the complex was collected and the data quality was assessed . The accessible data were checked for appropriate reliability if they were obtained using standard methods and had updated activity data including a comparison of references and calculation values. All estimations were based on widely accepted methods using data based on standardized measurement methods, and calculations using internationally accepted emission factors. The most suitable emission factors and speciation profiles for the various processes were selected from reputable literature sources and estimation of BTX emission load determined.

All potential stationary sources in the area were surveyed and it was determined whether they were sources of BTX. The locating and estimating of air emissions from sources of toluene, xylene and benzene and profiling of petroleum refineries were used as source identification guidelines[11,12]. Two refineries, four upstream petrochemical plants and all intermediate and downstream aromatics plants, as well as their storage areas were identified as potential sources and classified into area and/or point sources. Point sources include gas emitted through stacks of all potential sources, while area sources represent the fugitive emissions from processes, storage and distribution of petroleum raw materials and products. Stack parameters for point sources and locations of area sources were gathered from the Industrial Estate Authority of Thailand and were cross-checked against the data from monitoring reports. The emitted VOCs

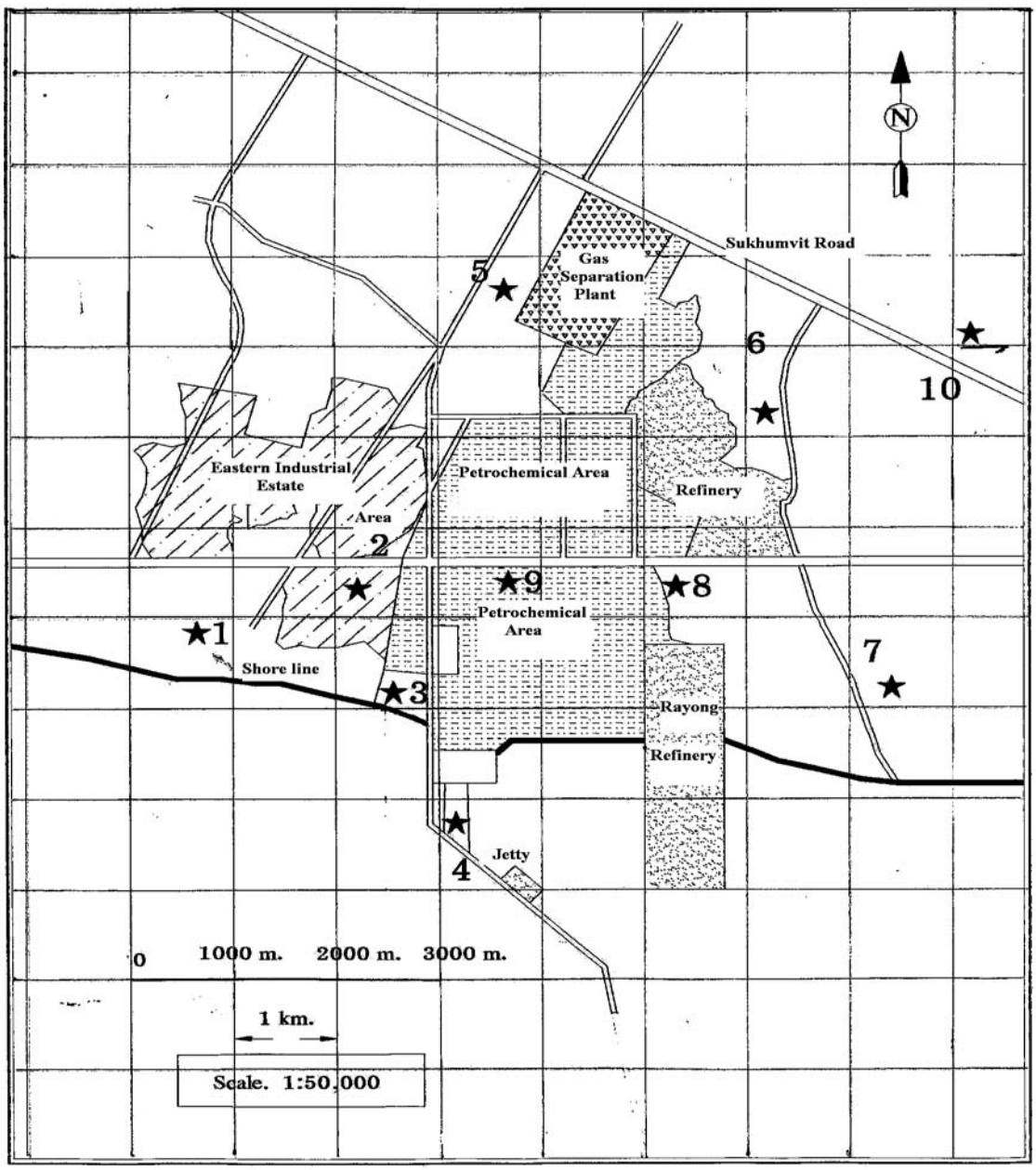


Fig 1. Map of Map Ta Phut Industrial Estate showing its Study Sites.
Note: 1= Nong Fab site; 2= Padaeng site; 3= IEAT site; 4= Jetty site; 5= SDC site; 6= School site; 7= THC site; 8= TSK site; 9= NFC site; 10= PAC site.

of each factory for both source types were collected from an Environmental Impact Assessment (EIA)[13,14], which has been approved by a National Committee set by the Office of Environmental Policy and Planning during the licensing process and its subsequent 6-monthly monitoring reports[15]. In this case, the estimation methods used were compared to reliable methods[16] and previous studies of VOCs in the area[17]. Annual activity data for all facilities were checked with the data reported by the Petroleum Institute of Thailand for the year 2000[18]. The VOC emission rates were adjusted as needed, and then, BTX speciation was done by applying speciation profiles of individual sources studied in some appropriate cases[19,20,21]. Data which already included estimated loads or fluxes for the targeted species and were in appropriate unit, g s^{-1}, were used directly as the emission loading from the identified sources. For data that needed to be calculated, the speciation loadings were estimated following equation 1.

$E_x = E_{voc}$ *Speciation factor *Conversion factor (1)

where: E_x = Emission rate of the species X in g s^{-1};

E_{VOC} = Emission rate of VOC in ton $year^{-1}$;

Speciation factor = weight % of VOCs released from each process operation

Conversion factor; 1 g s^{-1} = 0.0317 ton $year^{-1}$

In cases of direct estimation using emission factors and their annual production rates, the calculations were done using equation 2.

$$E_x = EF_x * Q \quad (2)$$

where: E_x = Emission of pollutant X;

EF_x = Emission factor of pollutant X; and

Q = Activity or annual production rates i.e., annual consumption of coal for power plant, annual production rates of petrochemical plants.

Line sources cover all traffic movement in and around the complex. These mobile sources included on-road vehicle emission but excluded non-road emission due to information and data limitations. These latter emissions were estimated to be quite minor. The vehicle kilometers traveled (VKT) method[22] was employed for estimating emission loads. The normalized emission was estimated using equation 3.

$$Q_k = \sum(VKT_i * EF_{ik}) \quad (3)$$

Q_k is emission rate of pollutant (k) in kg $year^{-1}$, VKT_i is the VKT of vehicle (i) in km $year^{-1}$, and EF_{ik} is the emission factor of pollutant (k) and vehicles (i), in kg km^{-1}. The traffic volume was based on a count by types of vehicles in the standard classes, heavy duty diesel (HDDV), light duty diesel (LDDT), light duty gasoline (LDGV) and motor cycle (MC) and modified using the increased rate of car registration reported by Land Transportation Department. Then, BTX speciation was done by applying speciation based on both exhaust and evaporative profiles of comparable individual vehicle types studied in Australia[23].

Source Modeling

The Industrial Source Complex Short-Term Version 3 (ISCST-3) model, developed by USEPA[24], was used to predict the added effects from the emission inventory for BTX on ground level ambient concentrations. The ISCST-3 model is a regulatory model that is widely used and accepted for the process of environmental impact assessment in Thailand. The model is capable of handling multiple sources, including point, volume, area and open pit source types. Line sources are modeled as a string of volume sources or as elongated area sources. Several source groups can be specified in a single run, with the source contributions combined for each group.

The ISCST-3 model for elevated continuous point sources uses the steady-state Gaussian plume equation given as equation 4.

$$C(x,y,z,H) = \left[\frac{Q_i}{2\pi u\sigma_y\sigma_z}\right]\left[e^{-\frac{y^2}{2\sigma_y^2}}\right]\left[e^{-\frac{(z+H)^2}{2\sigma_z^2}} + e^{-\frac{(z-H)^2}{2\sigma_y^2}}\right] \quad (4)$$

where Q_i is the emission rate from sources, u is the wind velocity, σ_y and σ_z are the dispersion coefficients in the horizontal (y) and vertical (z) directions, and H is the source height and plume rise. The model employs Brigg's formulae to compute plume rise, and it makes use of the power law to determine wind speed corresponding to the stack height. In general, the input to the model includes: (1) hourly meteorological data for wind speed, wind direction, ambient temperature, mixing height and stability class, (2) stack characteristics such as height, diameter, exit gas velocity, exit gas temperature and emission rate, and (3) co-ordinates of sources and receptors.

For area sources, the ISC area source algorithms were used to model low or ground level releases with no plume rise. The emission rate for an area source is an emission rate per unit area (g s^{-1} m^{-2}), which is different from the point and volume source emission rates, a total source emission. In cases of line sources, a string of volume sources, the ISC volume source algorithms are used. The volume emission rate in g s^{-1} and the initial lateral dimensions for line sources were input in the model. Choowichian[25] tested the sensitivities of the ISCST-3 model in the area based on SO_2 emissions. The SO_2 from point sources were input into the model under different meteorological conditions, such as different mixing height and stability classes. The model was found to work well and yielded reasonable outputs.

The surface meteorological data based on hourly

meteorological information for wind speed, wind direction and ambient temperature were obtained from the Nongfab station, which is located within the study area and is operated by IEAT. The three-hourly data measured at the study area for cloudiness were obtained from the Thai Meteorological Department. The dominant wind directions and maximum wind speeds during the study periods are 167-225 degrees and 3 m s^{-1} in February, 167-202 degrees and 2.5 m s^{-1} in April and 180-247 degrees and 3.5 m s^{-1} in June. The three-hourly measurements of the vertical temperature profile by radiosonde were obtained from the Pollution Control Department. Daily maximum temperature data and vertical temperature profile data were used to calculate the mean maximum mixing height on adiabatic diagrams and stability classes were classified following the Pasquill-Gifford method, which uses cloudiness and wind speed for nighttime and solar radiation and wind speed for daytime. The stack height characteristics and co-ordinates of sources and receptors were obtained from IEAT (Map Ta Phut Office). Both individual and combination complied annual average emission rates from mobile, point and area sources were used as inputs into the model. The output option in concentration mode was selected, as well as regulatory default in rural dispersion coefficient and options for deposition were turned off. The 1-hr average was selected for model calibration with measurement data and 24-hr and annual average options were selected for a worse case scenario. Three years, namely 2000, 2001 and 2002, of meteorological data were available. The worse case scenario modeling was based on the meteorological condition when dominant wind directions blew most frequently towards the residential area.

Results and Discussion

Emission Inventory

Based on the emission inventory methodology described, best estimated annual BTX emission loading from the Map Ta Phut locality were compiled and the results are shown in Table 1. For the three source types (point, line and area), it can readily be seen that area sources have the most potential impact on the ambient air. For the mobile (line) source, the BTX species were compiled at 0.47, 0.74 and 0.52 g s^{-1} for benzene, toluene and xylene, respectively, which gives a B:T:X relationship of 1:1.6:1.1. For point (stack) sources, which includes the power plants, emission rates of BTX have been determined as 3.08, 8.32 and 1.91 g s^{-1}, respectively, with a B:T:X relationship of 1:2.7:0.6. The highest emission loading in the Map Ta Phut complex comes from area sources, which contribute 13.64, 7.71 and 22.24 g s^{-1} for BTX, respectively, with a B:T:X relationship of 1:0.57:1.63. The most important point and area sources for BTX species are listed in Table 1. It is noticed that the emission of xylene was mainly from fugitive sources associated with the xylene production plants and refinery activities including the distribution and storage of their products. From this inventory, the fugitive emissions from tank farms, from the distribution and processes of refineries and from the upstream aromatic processes are seen to have the potential to

Table 1. Major Sources of BTX in the Study Area.

Item	Source Type	Processes	Speciation (g s^{-1})		
			Benzene	Toluene	Xylene
1.	Area	BTX Process Fugitives[d]	6.345	0.279	10.98
2.	Area	BT Process Fugitives[d]	4.597	0.97	NA
3.	Area	Refinery Tank Fugitives[f]	0.7	2.03	0.74
4.	Area	Refinery Valve & Fitting Leakage[f]	0.17	0.48	0.18
5.	Area	BTX Tank Fugitives[e]	0.08	0.023	1.91
6.	Area	Refinery Blow Down (1)[f]	0.01	0.012	0.005
7.	Area	Refinery Blow Down (2)[f]	0.009	0.011	0.005
8.	Point	Refinery Vapor Recovery Unit 1[a]	0.645	3.097	0.645
9.	Point	Refinery Vapor Recovery Unit 2[a]	0.645	3.097	0.645
10.	Point	Cogen-stacks[b]	0.459	0.085	0.013
11.	Point	Combined Stacks of Olefin Processes (1)[d]	0.43	0.68	NA
12.	Point	Combined Stacks of Olefin Processes (2)[d]	0.43	0.68	NA
13.	Point	Stacks of BT Processes[c]	0.251	0.418	0.473
14.	Point	Power plant combined stacks[b]	0.124	0.197	NA

NA= Not Applicable

[a] Direct measurement data from EIA monitoring report[15].

[b] BTX were estimated using emission factors based on raw materials used.

[c] BTX source profiles were multiplied with calculated VOCs using emission factors based on emitted gas reported in EIA main reports[14].

[d] BTX emission rates were estimated using emission factors based on annual rate of production.

[e] BTX source profiles were multiplied with VOCs data as reported in EIA[13].

[f] BTX source profiles were multiplied with VOCs data drawn from previous study[17].

contribute significant amounts of BTX to the airshed.

Source Modeling

The Industrial Sources Complex (ISCST-3) model has been used to predict the contributions of emissions from various sources to particular receptor sites. The model computed the effect of the compiled emission loading at each site, C, based on equation 4. For many conditions, the dispersion coefficients can be approximated by $s_y = Ax^{\alpha}$ and $s_z = Gx^{\gamma}$. Here x is the downwind distance (or travel time) and A, G, a, and g are empirically determined. For long downwind distances, the empirical terms in equation 4 will become ~1.0. If, in addition, it is assumed that u is relatively constant, then it can be found from equation 4 that

$$C \propto \frac{Q_i}{x^{\alpha+\gamma}} \qquad (5)$$

Here $1 \leq \alpha+\gamma \leq 2$. Consequently, if $\alpha+\gamma = 1$, the concentration should be proportional to the emission rate divided by the downwind distance from the source to the receptor (or travel time). The total concentration allocated to all sources at a particular receptor site is the sum of each of the emission contributions from upwind sources adjusted for distance. This was used to evaluate whether the BTX levels within the complex were higher than at downwind and residential sites.

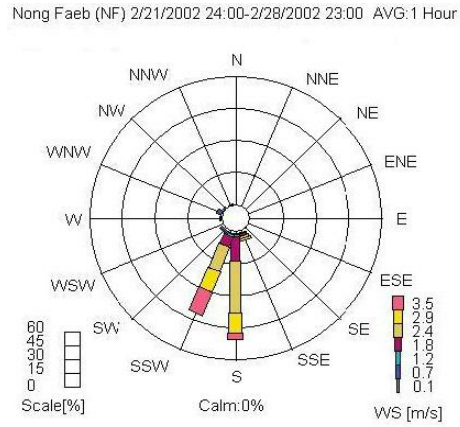
The seven receptor sites for the modeling are shown in Figure 1. They represent receptors within both the estate and nearby residential areas. Two sites, IEAT's office (IEAT, No.3) and Padaeng industry factory's guardhouse (Padaeng, No.2), represented the upwind region. The TSK's guardhouse (TSK, No.8) and National Fertilizer Company (NFC, No.9) were used as sites within the complex. Three community sites, downwind sites, were located at the Rayong Skills Development Center (SDC, No.5), the site of former secondary school (School, No.6), and the Ta Kuan Public Health Center (THC, No.7). Some additional sites at the Nong Fab monitoring station (Nong Fab, No.1), 3 kms west-southwest of the estate, and at the Provincial Administrative Center (PAC, No.10), 4 kms east of the estate, were used selectively to check the transportation of air mass from the estate. One further site at Thai Tank Terminal (Jetty, No. 4) was also selected to check spatial variation of BTX in the area.

The individual source loading and total loading of BTX were simulated for three periods each of one-week, namely the dry (22-28 February), the semi-wet (29 April- 5 May) and the wet season (19-25 June) in 2002. These periods occurred when winds were coming predominantly from the sea and downwind impacts from emissions would be on neighboring residential areas. The wind rose diagrams for all three monitoring periods are shown in Figure 2.

The modeling results indicated that mobile source emissions contributed to ambient concentrations at all monitoring sites, whereas point and area sources sometimes made no contribution but did, on occasion, play a much more significant role than mobile sources in affecting the ambient concentrations. At the industrial sites, TSK and NFC, which are within the complex and located near the sources, the BTX concentrations were dominated mainly by area sources (See Table 2 for the TSK site). The downwind sites, SDC and the school, also showed evidence of the impacts from point and area sources. Some results are shown in Table 3 for benzene and toluene at the school site for period 2. From the modeling predictions, the additional contribution from area and point sources to these downwind sites is generally in the range of 3-10% for benzene and 4–20 % for toluene, but can be, on occasions, as high as 30% for benzene and 60% for toluene. The BTX concentrations at two upwind site, IEAT and Padaeng and at the THC site were only occasionally affected by point and area sources. The

Table 2. Modeled Concentration Data and Corresponding Measured Data at TSK Site for Selected Days.

Date	Benzene						Toluene					
	Predicted Values					Measured Values	Predicted Values					Measured Values
	Line	Point	Area	Total load	Higher load		Line	Point	Area	Total load	Higher load	
22/2/02	0.18	0.19	3.0	3.4	45.5	32.1	0.3	0.23	31.7	32	102.6	220.8
23/2/02	0.21	0.26	2.1	2.6	42.3	7.3	0.4	0.03	23.1	23.5	111.7	110
25/2/02	0.28	0.47	2.0	2.7	3.2	5.3	0.31	0.8	7.6	8.7	25.5	77.9
1/5/02	0.04	0.37	0.3	0.7	7.8	5.9	0.66	0.43	1.4	2.5	4.1	3.1
3/5/02	0.17	0.47	2.7	3.4	3.4	3.8	0.39	0.95	6.3	7.7	7.8	5
4/5/02	0.00	0.44	2.9	3.3	10.8	16.9	0.00	3.28	12.0	15.3	33.4	23.3
19/6/02	0.30	0.00	4.6	4.9	16.2	4.8	0.46	0.00	22.1	22.6	45.3	8
20/6/02	0.24	0.5	2.9	3.6	25.3	3.4	0.48	0.15	26.0	26.6	149.4	83.4
23/6/02	0.35	1.75	4.4	6.5	7.7	4.9	0.59	2.73	1.2	4.5	4.6	4.4



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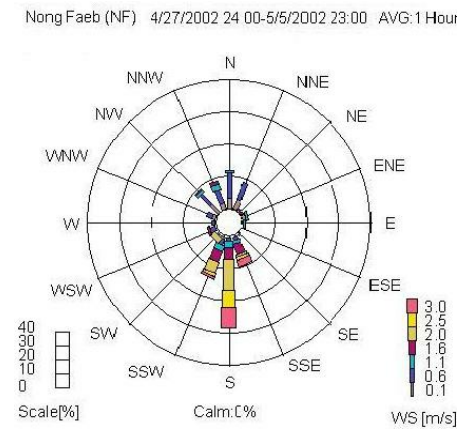

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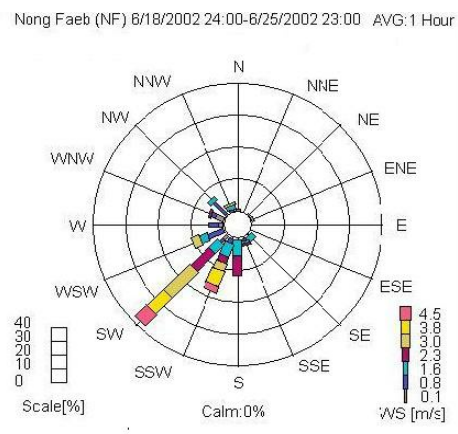

(c)

Fig 2. Wind Rose Diagrams during three sampling periods at Nong Fab station; (a) 21-28 February 2002, (b) 27 April-5 May 2002, and (c) 18-25 June 2002.
Source: Industrial Estate Authority of Thailand (Map Ta Phut office) 2002.

Table 3. Predicted and Measured Values at School and THC Site during Monitoring Period #2.

Date	Site	Benzene, μg m^{-3}						Toluene, μg m^{-3}					
		Line	Point	Area	Total load	Predicted*	Measured	Line	Point	Area	Total load	Predicted*	Measured
30/4/02	6	0.08	0.00	0.00	0.1	3.2	3.8	0.12	0.00	0.3	0.4	2.9	2.6
	7	0.13	0.00	0.00	0.1	3.2	3.2	0.2	0.00	0.00	0.2	2.7	3.7
1/5/02	6	0.09	0.00	6.1	6.8	10.0	3.7	0.14	0.00	4.1	4.3	6.8	2.1
	7	0.09	0.00	5.2	5.3	8.4	4.9	1.48	0.00	2.0	3.5	5.6	3.5
2/5/02	6	0.12	0.00	0.00	0.12	3.2	6	0.19	0.00	0.00	0.2	2.7	4.1
	7	0.13	0.00	0.00	0.1	3.2	4.8	0.11	0.00	0.06	0.2	2.7	7.9
3/5/02	6	0.05	0.00	0.07	0.12	3.2	3	0.07	0.00	2.1	2.2	4.7	2.3
	7	0.06	0.00	0.5	0.6	3.7	4.9	0.09	0.00	0.46	0.5	3.0	5.7
4/5/02	6	0.37	0.00	0.5	1.0	4.1	5	0.53	0.00	2.50	3.0	5.5	7.1
	7	0.08	0.00	0.00	0.1	3.2	7.2	0.15	0.00	0.00	0.1	2.6	8.7
5/5/02	6	0.08	0.00	0.05	0.6	3.7	7.2	0.09	0.00	0.2	0.3	2.8	5.6
	7	0.05	0.00	0.15	0.2	3.3	5.5	0.08	0.00	0.10	0.2	2.7	2.8

Site 6 = School site, Site 7 = THC site.
*Predicted Values = Total modeled values plus background concentrations (3.1 μg m^{-3} for Benzene and 2.5 μg m^{-3} for Toluene).

predicted and measured values for the THC site are also shown in Table 3. This table also highlights the relative importance of the three source types (line, point and area) for the individual modeling.

Comparison of Computed Results and Measurement Data

In order to verify the model predictions, direct measurement of air quality, having better inherent credibility, was used. Air samples for analysis were collected at the selected sites for the three study periods in February, April and June 2002. Samples were collected on 7 consecutive days for each period. The sampling was conducted at one meter above ground level using a calibrated low flow pump (SKC Model 224-PCXR8) at flow rate 0.1 litre min^{-1} for 100 min into tubes containing charcoal (SKC No. 226-09). The trapped BTX members were desorbed with 1 ml of carbon disulfide (purified and re-distilled) and analyzed by gas chromatography equipped with a flame ionization detector (GC/FID-Model Varian CP-3800). Performance criteria included method detection limits, standard calibration curve, breakthrough testing, % recovery, precision testing, and field and laboratory blanks. For modeling purposes, background ambient concentrations of 3.1, 2.5 and 1.7 μg m^{-3} for benzene, toluene and xylene respectively, have been adopted. These values are based on averaging across the upwind and reference sites.

Comparisons between model predicted and measured values at the selected sites have been made. For the industrial sites and the downwind sites, the correlation coefficients for measured and predicted data are 0.76 (n = 62) and 0.35 (n = 66) respectively, with 72% of data points falling within a factor of two. The coefficients of determination (R^2) for the industrial, downwind and upwind sites are 0.58, 0.13 and 0.12, respectively. The scatter plot of the best correlation at two industrial sites with R^2 equals 0.58 is shown in Figure 3. This implies that there is little relationship between the measured and predicted values at the upwind and downwind sites, while 58% of the variability observed within the complex can be explained by the model. The findings point to the situation that particular nearby sources caused the ambient concentration of BTX at the industrial sites to be higher than at the downwind sites. It was found that the BTX within the complex was high when the relative distances of these sites from sources were considered, which was previously discussed with respect to equation 5. There is a slight tendency for the model to over predict average levels and under predict high episodes. There is some debate in the factory documentation for the refineries concerning the adequacy of the loading associated with fugitive emissions. Some modeling using much larger emissions have been made and the predicted values at the two industrial sites were observed to be quite source strength dependent whereas values at

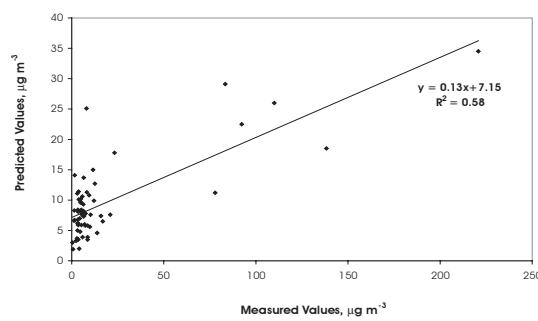

Fig 3. Scatter Plot of Predicted and Measured Values for BTX at Two Industrial Sites.

downwind sites are were affected little. This is to be expected with ground level area emissions. With the higher fugitive loads, the coefficients of association between measured and predicted values of the modeling calculation decreased from R = 0.76 (R^2 = 0.58) to R = 0.65 (R^2 = 0.42), but there was no significant impact on values associated with the downwind sites.

It can be seen in the emission inventory that xylene has more limited sources and hence modeling of this species should display less variability. A comparison of measured and predicted values at the TSK site, which is geographically close to the dominant xylene source, shows some association with R=0.6 and 60% of data fall within a factor of two. The xylene level at the other downwind and upwind sites showed a very low or BDL reading from the BTX measurements.

From the predicted and monitoring data, it was seen that benzene showed slight over-prediction in both industrial and downwind areas while toluene exhibited slight under-prediction in both areas. A good comparison was observed between the predicted and measured Xylene concentrations at the two industrial sites. The comparisons between the measurement and modeling results within the complex are quite respectable and attest to the value of the emission inventory and modeling approach.

Predicted Annual Concentrations of BTX at Study Sites

Using the meteorological data for the year 2002, a worse case scenario when the winds blow most frequently toward the residential area, together with the compiled emission inventory, has been simulated. The results, based on line sources and combined stationary sources at the study sites, are shown for individual BTX species in Table 4. For this exercise, no airshed background concentrations were added. It was found that line sources contributed small amounts to the predicted annual concentrations at all monitoring sites except the PAC site. The TSK, school and NFC were found to have relatively high contamination when compared to other sites. This is due to the locations of these sites at the downwind direction from the major sources. The concentrations of individual species were compared to ambient air quality standard and health benchmark[26,27]. It was found that the annual predicted benzene at three sites, TSK, School and NFC, did not exceed the WHO guidelines of 16.2 μg m^{-3} (5 ppbv) and were lower than the value associated with possible chronic effects of 60 μg m^{-3}. Both toluene and xylene were well below any chronic effects level, which are set at 400 and 700 μg m^{-3} respectively. Consequently, the TX hourly average standards set at 4400 and 5400 μg m^{-3} and their 24-hr averages at 3000 and 3500 μg m^{-3} are considerably higher than the predicted values.

Table 4. Computed Annual Average Concentrations at Monitoring Sites based on (1) Stationary Sources, (2) Line Sources.

Site	Benzene		Toluene		Xylene	
	(1)	(2)	(1)	(2)	(1)	(2)
SDC	3.7	2.7	4.1	4.2	6.6	3
School	9.1	0.8	28.1	1.2	12.7	0.9
THC	0.5	1.0	2.9	3	0.3	1.2
TSK	10.3	0.5	30.4	0.8	23.7	0.6
NFC	9.3	0.5	17.2	0.8	22.8	0.6
IEAT	4.9	0.3	7.6	0.5	10.2	0.4
Padaeng	3.6	0.2	6.7	0.4	7.2	0.3
Jetty	6.7	0.3	10.2	0.4	14.1	0.3
PAC	0.3	1.3	0.6	1.9	0.6	1.4
NongFab	2.3	0.3	6.1	0.5	5.1	0.3

Unit = mg m^{-3}.
Computed values for (1) and (2) excluding background concentrations.
Chronic benchmarks for BTX are 60, 400 and 700 mg m^{-3}, respectively.

Conclusion

The emission inventory results demonstrate the overwhelming importance of area sources for the ambient air in and nearby the complex. The ISCST-3 air dispersion model, which is widely regarded as capable of providing conservative estimates, was used to identify the effects of the compiled emission loading in the area. The predicted values were compared with the measured values and reasonable associations were found across the BTX ambient concentrations. It was observed that the stationary industrial sources, through either process related or tank farm fugitive emissions, dominated the ambient concentrations of target species.

As a general rule, model impacts are more accurate for the following: longer averaging periods, sources with well-defined emissions and release characteristics, and receptor areas that do not experience steep concentration gradients. The validity of any air quality model results depends on the quality of input data. Air pollutants' emission rates that are grossly underestimated will produce modeled impacts that are also grossly underestimated. Since the estimation of emissions is often uncertain, these uncertainties should also be taken into account when reviewing and taking action based on model predictions.

Sources parameters have been carefully evaluated and specified as accurately as possible in this study. While acknowledging the limitations with regard to the modeling method and the uncertainties associated with the emission data[28], the results found from this study have value for regulatory agencies in setting up emission standards either for point or area sources of the species in the area. Consequently, policy makers should be able to make use of these findings in planning to manage the

emission sources and their impacts in the area.

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