A MODEL FOR PRIORITISATION OF INDUSTRIAL AIR POLLUTANTS: PART I. FORMULATION

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ABSTRACT

This paper describes the formulation of a prioritisation model applied to industrial toxic air pollutants released into the atmosphere through stack and fugitive emissions. This model takes into consideration the relative toxicity of a range of commonly used industrial chemicals, volume released into the air, contaminant transported in the plume, and atmospheric fate of chemicals. The key features of model include Nearby Population Exposure Index (PEI), Occupational Exposure Index (OEI), and Chemical Health Risk Index Number (CHRIN). The approach is to quantify in a relative sense, the potential health risks of nearby population and in-plant workers. The model, when applied to any manufacturing facility that releases toxic chemicals into the air would produce a rank-ordered list of CHRIN. The higher the CHRIN, the more problematic is the chemical. The model is intended to help a particular manufacturing facility devote its resources more effectively to environmental air pollutants control strategies and research on toxic use reduction technologies and methods, or prioritise the facility's research agenda in toxics use reduction.

Keywords : *Chemical Health Risk Index Number (CHRIN), Fugitive Emissions, Industrial Air Pollutant, Model, Population Exposure Index (PEI), Prioritisation, Occupational Exposure Index (OEI), Relative Toxicity, Stack Emissions*

1 INTRODUCTION

Different toxic chemicals can exert different health effects and environmental impacts. For instance, toxic chemicals released from a facility can differ in the degree of toxicity or their persistence in the environment [1]. More importantly, a facility can release quantities of a variety of chemical compounds into various environmental media [1]. However, merely accounting for the volume of release of pollutants does not completely reflect the varying impacts on nearby population, in-plant workers, and the environment as a whole. In fact, the health hazard risks to the nearby population and in-plant workers posed by the individual toxic chemicals emitted into the atmosphere from a facility are a function of: (a) relative toxicity of chemicals; (b) volume released; (c) contaminant transported in the plume; (d) atmospheric fate of chemicals; and (e) meteorological conditions over the facility [1].

To date, a quantitative method incorporating these factors for analysing health risks due to environmental releases into the atmosphere does not exist [1]. Some related work previously done by the National Institute for Occupational Safety and Health (NIOSH) and United States Environmental Protection Agency (USEPA) form the backbones of this model formulation. The National Occupational Hazards Survey (NOHS), which was conducted by NIOSH during 1972-1974 in approximately 5,000 industrial facilities, generated data which was later used to estimate the number of workers potentially exposed to particular chemical compound and to estimate the extent of worker exposures in the workplace [2]. In addition, the database entitled "The Registry of Toxic Effects of Chemicals Substances" (RTECS), developed by NIOSH that summarises all of the chemical-specific toxicity studies available in the published technical literature [3]. NIOSH scientists attempted to use the 1972-1974 NOHS and 1981 RTECS files for the purpose of quantifying in a relative sense, potential health risks associated with industries and occupations covered in NOHS [4]. Pedersen et al. [4] developed a model entitled "A Model for the Identification of High Risk Occupational Groups using RTECS and NOHS Data", which was published in October 1983. The model was designed to produce rank-ordered lists of exposures to chemical compounds in various industries and occupations. The chemical Hazard Risk Index (HRI) contained in the models is an integral part of this research. HRI is a listing of chemical compound indices (including metals and inorganic compounds) common to both the 1982 RTECS [3] and 1977 NOHS [2] databases as well as selected data from United States Bureau of the Census [5], ranked by the toxicological risk they pose, and the numbers (HRI) are indicative of the chemical risk [4]. The higher the numerical value of HRI, the higher toxicological risk a chemical poses. Even though HRI is based entirely on the unevaluated animal studies toxicological data available in the RTECS, it is the only known reasonable guide in estimating the relative toxicity of a wide variety of organic and inorganic chemical compounds [4].

Since 1987, documentation of the levels of various toxic chemicals emitted from a facility to the environment, that is, air, water, land, underground injection and off-site location transfers, has been conducted by the EPA, following the enactment of the "Superfund Amendments and Re-authorisation Act of 1986" or SARA Title III [6]. The act requires a facility to report to the USEPA the amount of certain toxic chemicals released to the environment during the past calendar year. In addition, the facility must report the quantities of both routine and accidental releases of the listed chemicals, the maximum amount of the listed chemicals on-site during the calendar year and the amount contained in the waste transferred off-site [6]. The information is made available to the public through on-line computer searches of the Toxic Chemical Release Inventory [7] database at the National Library of Medicine (NLM, MEDLARS). Some of the information regarding environmental releases includes stack emissions, fugitive emissions, releases to surface water bodies, publicity owned treatment works (POTW), underground injection, land, and off-site location transfers. Thus, both the stack and fugitive emissions into the atmosphere, the only considerations in this model formulation exercise, are readily available. Fuller et al. [8] prepared a research paper for USEPA entitled "Preliminary Scoring of Selected Organic Air Pollutants" outlining a methodology of ranking organic air pollutants entering the atmosphere form industrial sources. In this study, three parameters were taken into consideration for this ranking system: (a) volume of release from a facility; (b) volatility of the pollutant; and (c) chemical toxicity. Their total toxicity scoring method serves as important reference in this model development for assigning "weights" or "multipliers" for acute toxicity, carcinogenicity, equivocal tumorigenicity, mutagenicity, neoplasticity, primary irritation, teratogenicity, etc. while calculating the Health Risk Index Number [8].

Howard et al. [9] compiled a complete range of rate constants for individual abiotic and biotic degradation for chemicals of anthropogenic origin present in soil, water and air. Estimates were performed for chemicals in which rate constants could not be located in the available literature. A range of half-lives (in hours) were estimated for degradation in soil, water and air which do not account for the transport of chemicals between environmental compartments, and all the 331 chemicals covered by the SARA Title III were included [6], [9]. The half-lives in the air serve as the chemical atmospheric fate or atmospheric persistency in this research project, which were then converted to Chemical Atmospheric Fate Index (CAFI) [10-11].

In-plant workers exposure was estimated by categorisation of employees into full-time and part-time to allow for differing lengths of exposures, and calculating the predicted workplace contaminant concentrations. All fugitive emissions were assumed to take place within the facility and chemicals are assumed to airborne. In addition, weights of the index given to full-time and part-time exposures would be the average of NIOSH's and OSHA's rating systems. The unit for Occupational Exposure Index (OEI) is in person-part per million or person-ppm [12].

2 PRIORITISATION MODEL

One of the primary components of this prioritisation model is the volume of the pollutants released into the air through stack. The other factors include relative toxicity of air pollutants, the hourly and daily meteorological conditions, nearby population exposure around the facility, in-plant workers exposure, and chemical atmospheric fate. Figure 1 illustrates the index production data flow diagram that summarises the integration of individual factors into the air pollutants prioritisation model. This model is primarily an integration of some of the major components such as: (a) relative toxicity of air pollutants released; (b) meteorological

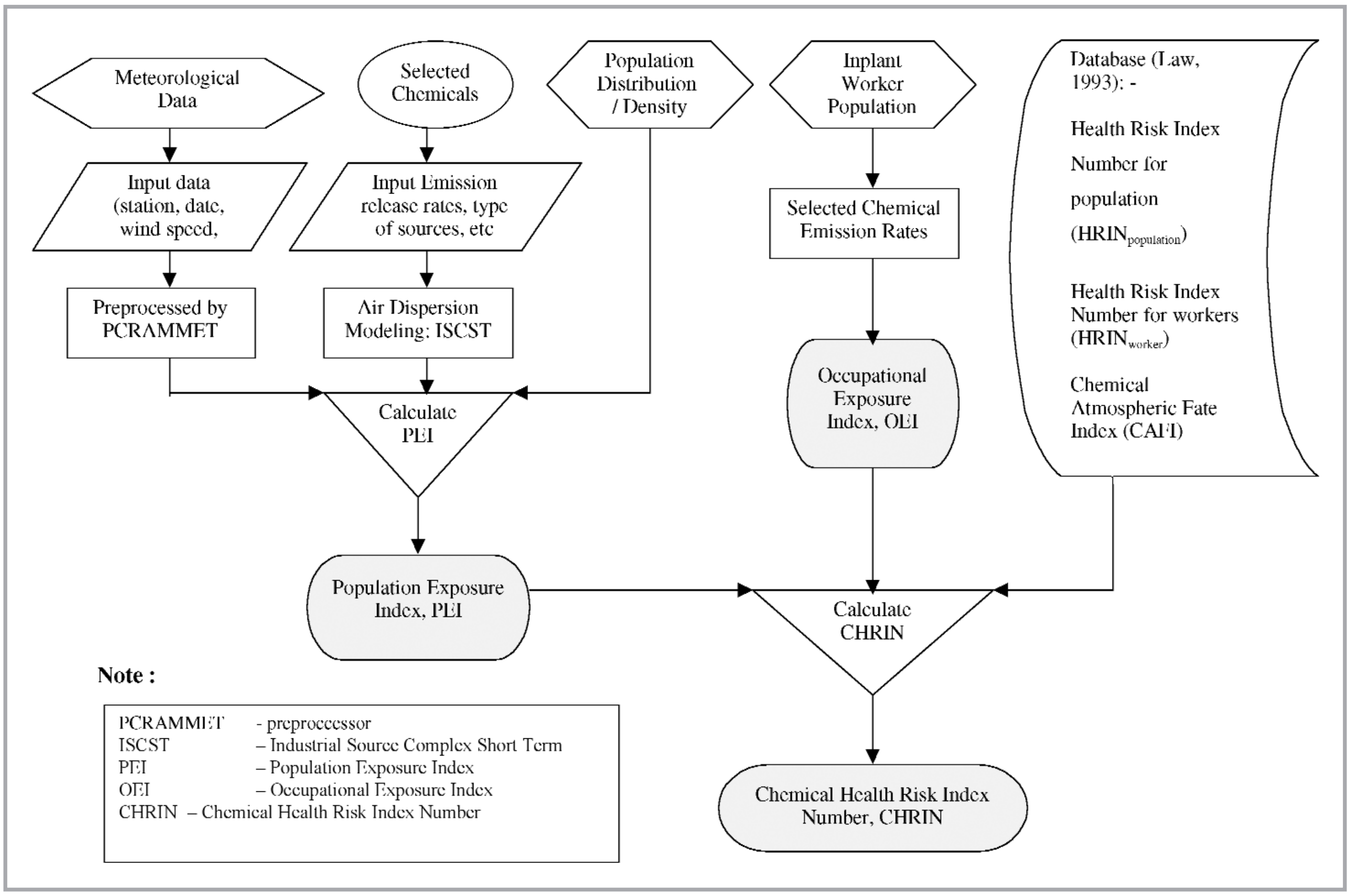

Figure 1: Index production data flow

data; (c) atmospheric air dispersion model; (d) PCRAMMET; (e) nearby population exposure; (f) occupational exposure; (g) Health Risk Index Number for population ($HRIN_{population}$); (h) Health Risk Index Number for workers ($HRIN_{worker}$); and (i) Chemical Atmospheric Fate Index (CAFI). The model is designed to produce Population Exposure Index (PEI), Occupational Exposure Index (OEI), and Chemical Hazard Risk Index Number (CHRIN).

2.A METEOROLOGICAL DATA

The meteorological conditions over the industrial facilities or industrial zone include the mean surface air temperature; mean and maximum surface wind speed and direction obtainable from Malaysian Meteorological Service. The ISCST air dispersion model is chosen as one of the key components of this model that uses the meteorological information on an hour-by-hour basis. The ISCST air dispersion model is deemed a suitable for assessing pollutant concentrations from the wide variety of sources associated with industrial complexes in SJFIZ [13-14]. The hourly weather data contains wind speed, wind direction, temperature, atmospheric stability, and mixing heights [15-16].

2.B PCRAMMET

PCRAMMET is a pre-processor program that provides and merges all the data such as hourly stability class, wind direction, wind speed, ambient temperature and mixing height for use in ISCST [15-16]. It processes five input data formats which are: (a) hourly surface observations; (b) twice-daily mixing height data; (c) hourly surface observations; (d) hourly surface observations; and (e) precipitation data. The data input files for running PCRAMMET are mixing height data and hourly surface meteorological data. For pollutant concentration estimation, the necessary mixing height data required are National Weather Service (NWS) Station Number, year, month, day, morning mixing height values and afternoon mixing height values [15-16]. All those data are arranged in a specified column in a file with extension *.mix*. The variables used by PCRAMMET are NWS station, year, month, day of record, hour, ceiling height, wind direction, wind speed, dry bulb temperature, total cloud cover and opaque cloud cover. Those data are properly arranged in a file with extension *.srf* [15-16].

The data offered in the mixing height data files are comprised of data provided by the Malaysian Meteorological Service in their "Twice Daily Mixing Height Data" format. The format of the records has been modified to correspond to that required by the PCRAMMET pre-processor programs. In addition, the first and last records of each file have been added to conform to the requirements of these pre-processor programs. PCRAMMET also require that the meteorological input data sets contain no missing values [15-16].

The processing of hourly mixing heights requires morning and afternoon estimates of mixing heights, the local standard time of sunrise and sunset and hourly estimates of stability. Two Interpolation schemes are used to estimate hourly mixing heights, one for rural sites and the other for urban sites. Both estimates are included in the PCRAMMET output file. The time of sunrise and sunset are calculated within PCRAMMET based on the date, latitude, longitude, and time zone, using known earth-sun relationships [15-16].

2.C ATMOSPHERIC AIR DISPERSION MODEL

Industrial Source Complex Short-Term (ISCST) was developed by United States Environmental Protection Agency (USEPA) and is a regulatory model for both State and Federal government of the United States of America [17]. The ISCST air dispersion model is a steady-state plume model, which can be used to assess pollutant concentrations from wide variety of sources, associated with an industrial source complexes. This model can account for settling and dry deposition of particulate, downwash, area, line and volume sources, plume rise as a function of downwind distance, separation of point sources, and limited terrain adjustment [15-16]. The ISCST is designed to calculate the average seasonal and/or annual ground level concentration or total deposition from multiple continuous point, volume and/or areas sources [15-16]. Provision is made for special discrete, X, Y receptor points that may correspond to sampler sites, points of maximum or special points of interest. Some of the major factors considered in analysing air quality impacts of emissions from industrial source complexes are stack emissions, hourly meteorological information, and time-dependent exponential decay of pollutants, dry deposition, and gravitational settling [15-16].

2.D POPULATION EXPOSURE INDEX (PEI)

Population Exposure Index (PEI) is a listing of population exposure indices ranked by the potential exposure to chemicals. The exposure of the population in the proximity is a function of size and contaminant levels of the plumes [12]. An area in the proximity covered by the plume and with pre-determined average population densities of each individual area can be approximated from the isopleths plotted. The sum of all the products of the individual area covered by plume would produce a Population Exposure Index (PEI) in persons milligrams/micrograms per cubic meter (person-$\mu g/m^3$) that could be converted to person parts per million (person-ppm). The PEI sums the risk associated with each of the toxic chemicals to which population in the nearby facility or facilities are potentially exposed as follows [12]:

$$\text{PEI} = D(C_1A_1+C_2A_2+C_3A_3+ \text{........} +C_nA_n) \text{ person-ppm} \quad (1)$$

in which D = population density distributions (persons/km^2); C_i= pollutant concentrations (ppm or $\mu g/m^3$); A_i = plume covered areas (km^2); and i = 1 to n (where n is the number of census tracts).

2.E OCCUPATIONAL EXPOSURE INDEX (OEI)

Occupational Exposure Index (OEI) is a listing of chemicals ranked by potential chemical risk to workers in the facility under study. The algorithm that produces this index is intended to calculate the incremental risk posed by each chemical to which workers in a facility are potentially exposed. The Occupational Exposure Index calculation for any given chemical compound found in a given facility is based on the expression below [12]:

$$\mathrm{OEI} = 0.095\ C_f(pen)\ (0.222+0.778p_f)\ \text{person-ppm} \qquad (2)$$

where C_f = calculated pollutant concentration in the facility; *pen* = total number of employees in the facility; and p_f = percentage of full-time exposures.

2.F.1 ESTIMATION OF IN-PLANT CONCENTRATION (C_f)

One of the primary factors in determining the rate of contaminant build-up or respective contaminant levels in a facility is the type of exhaust ventilation installed [18]. To facilitate calculations of contaminant levels in the facility due to vapor pressures or volatilities of chemical compounds, the targeted facility buildings are assumed to be equipped with general exhaust ventilation, also called dilution ventilation systems, which is typical for most industrial plants [18].

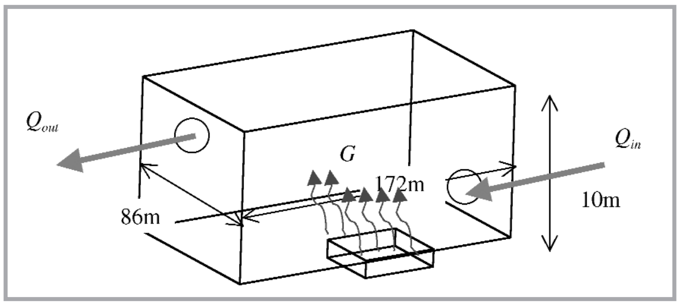

Figure 2: Nominal building structure

A single model of the facilities is illustrated in Figure 2. The box represents the typical physical structure of the facilities under study, with the fugitive emission rate (*G*) in grams/second (g/s), the volume of the building (*V*) in cubic meters (m^3), and the air is exhausted at a volumetric rate (*Q*) in cubic meters per second (m^3/s). The key element in a general exhaust system is usually a propeller-type exhaust fan mounted in the wall or ceiling, with no extensive exhaust ductwork system involved. Even though the fresh air or replacement air could be supplied in various ways, a typical supply of air is provided by natural infiltration of ventilation. For predicting general exhaust ventilation performance, which in terms would determine the contaminant levels with the facility, several assumptions must be made as follows [12]:

(a) the pollutants' generation rates are constant;
(b) there is steady-state concentration of each pollutant;
(c) the pollutants are removed from the facility solely via general exhaust ventilation;
(d) there is perfect mixing of pollutants and air in the facility, and thus, the factor for complete mixing (K) is equal to one [18];
(e) the exhaust ventilation rate is 10 air changes per hour [18];
(f) inhalation is the only route of exposure;
(g) air contaminant concentration is equivalent or at least proportional to dose delivered to the lungs and into the blood system; and
(h) dose concentration from source exposures is not considered in this model.

This is aimed at determining annual average concentrations to which workers are potentially exposed for the individual chemical compound emitted within a facility as fugitive emissions. With known ventilation rate (*Q*) and a contaminant generation rate (g/s), a constant concentration (mg/m^3) could be derived by starting with a basic material balance equation [12].

Referring to the model in Figure 2, the rate of accumulation is the nett value of the rate of generation minus the rate of removal as follows:

$$VfC_f = Gft - Q'C_f\ \partial t \qquad (3)$$

in which *V* = volume of building (m^3); *G* = generate rate (g/s); Q_{in} = amount of replacement air (m^3/s); Q_{out} = amount of exhaust air (m^3/s); C_f = concentration of pollutant, gas or vapour (g/m^3); and *t* = time (s).

At a steady state,

$$fC_f = 0 \qquad (4)$$

Substituting Equation (4) into Equation (3) gives

$$Gft = Q'C_f ft \qquad (5a)$$

Therefore,

$$Gft = Q'C_f ft \qquad (5b)$$

Hence,

$$G = Q'C_f \qquad (5c)$$

Solving for C_f gives

$$C_f = \frac{G}{Q'} \qquad (5d)$$

To account for incomplete mixing within the facility, a *K* value ranging from 1 (perfect mixing) to 10 (poor mixing) is introduced to modify the rate of ventilation [18], and thus

$$Q' = \frac{Q}{K} \qquad (6)$$

where *Q* = actual ventilation rate (m^3/s); Q' = effective ventilation rate (m^3/s); and *K* = a factor to allow for incomplete mixing.

Substituting Equation (6) into Equation (5d) gives

$$C_f = \left(\frac{G}{Q}\right)\mathrm{K} \qquad (7)$$

In this model, a default size of a nominal manufacturing facility is (172m x 86m x 10m) = 147 920 m^3, and the air change rate per hour (ACPH) is calculated to be approximately

10 [19-20]. Thus, the actual ventilation rate, Q is [147,920 / (10 x 60min x 60s)] = 4.1089 m^3/s, and by substituting the K value of 1 (perfect mixing assumed) and Q value of 4.1089 m^3/s into Equation (7), the in-plant concentration of pollutants C_f becomes

$$C_f = \frac{G}{4.1089} \quad g/m^3 \qquad (8)$$

Concentrations of pollutants can be expressed in units of mass per unit volume ($\mu g/m^3$, micrograms per cubic meter) or in terms of a volumetric ratio (ppm, volume of contaminant per million volumes of air) [21]. The conversion between mass units and volumetric ratios at standard temperature and pressure is approximated by

$$\text{ppm} = \frac{\mu g/m^3 \longleftrightarrow 0.02445}{MW} \qquad (9)$$

in which MW = molecular weight of contaminant (grams/mole).

2.F HAZARD RISK INDEX NUMBERS (HRIN)

$HRIN_{population}$ and HRINworker are two individual lists of chemical indices ranked by the toxicological risk they pose on the nearby population ($HRIN_{population}$) and in-plant workers ($HRIN_{worker}$) [12]. The HRIN is an indication of the relative toxicological risk posed by each chemical. These numbers are to be used to prioritise the chemicals in the index. The HRIN is based upon the animal study toxicological data available in RTECS and the characteristics of exposure, that is, chronic or acute [12].

2.G CHEMICAL ATMOSPHERIC FATE INDEX (CAFI)

CAFI is a listing of indices for the estimation of time for degradation of a chemical compounds in the atmosphere to half of their concentrations. Oxidation and/or photochemical degradation are the major sources in the atmosphere; the reactions most frequently considered are those with hydroxyl radicals (OH) and with ozone (O_3) in a first-order reaction [12].

2.H CHEMICAL HAZARD RISK INDEX NUMBER (CHRIN)

CHRIN could be finalised with the combination of Health Risk Index Number (HRIN), Chemical Atmospheric Fate Index (CAFI), Population Exposure Index (PEI), and Occupational Exposure Index (OEI). CHRIN are then used to prioritise and rank the given toxic chemicals emitted into the atmosphere. CHRIN may be written as follows [12]:

$$\text{CHRIN} = [J_1 \text{HRIN}_{\text{POPULATION}} + J_2 \text{CAFK}(K_1 \text{PEI})] + [(K_2 \text{OEI})(J_1 \text{HRIN}_{\text{WORKER}})] \qquad (10)$$

where $HRIN_{population}$ = Health Risk Index Number for population; $HRIN_{worker}$ = Health Risk Index Number for workers; CAFI = Chemical Atmospheric Fate Index; PEI = Population Exposure Index; OEI = Occupational Exposure Index; and J_1, J_2, K_1, K_2 are indicate variable numerical factors (weights) for the enhancement or suppression of individual sub-indices.

Chemical Hazard Risk Index Number (CHRIN) is used to prioritise and rank the given toxic chemicals emitted into the atmosphere as represented by Equation (10). In calculating the CHRINs, it needs to properly weight the PEI and OEI. It seems reasonable to multiply the OEI by 0.238, because workers are exposed to 8 hours per day, 5 days per week (total of 40 hours per week) as compared to the general population exposures of 24 hours per day, 7 days per week (total 168 hours per week) [12]. Therefore, K_1 and K_2 may be given a value of 1 and 0.238, respectively [12]. Generally, it is conservatively assumed the chemical toxicity (HRIN) is much more problematic than the chemical atmospheric persistency (half-life). Therefore, in this study, J_1 (weight of HRIN) is given a weight 5 times that of J_2 (weight of CAFI) [12]. It was found that the wide variation in worker and population indices (OEI and PEI) within the individual facilities could be as much as four significant figures. To bring the range of indices into more manageable terms, the indices were converted to a logarithmic scale. This produced indices that were all below 10, while maintaining the capability to recognise small differences that exist among some of the population exposure indices. Then Equation (10) may be rewritten as follows [12]:

$$\text{CHRIN} = \log[(5\text{HRIN}_{\text{POPULATION}} + \text{CAFI})(\text{PEI}) + 0.238(\text{OEI})(5\text{HRIN}_{\text{WORKER}})] \qquad (11)$$

3 CONCLUSIONS

The prioritisation model applied to industrial air pollutants emitted through stack and fugitive emissions could serve as a useful tool to any individual or a group of industrial manufacturing facilities intending to identify and prioritise the air pollutants, and effectively to devote its research effort or research on toxics use reduction technologies and methods. The chemical health risk indexes generated from model algorithms serves as a valuable reference in prioritisation of industrial pollutants released into the atmosphere. ■

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