Quantifying potential off-site impacts of SARA Title III air releases

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Abstract

SARA Title III has resulted in the development of an air toxics emissions data base that can be used to evaluate, manage and reduce the potential for off-site health risks. A general procedure is described to efficiently conduct off-site impact assessments using a step-wise approach. Adoption of these guidelines will result in a consistent basis of evaluation among many sites and substances which is especially important when evaluating corporate-wide air toxics impacts. The analysis steps include selection of ambient exposure criteria, ambient air quality screening, refined modeling and risk assessment. A case study application illustrates the utility of the methodology.

Introduction

The advent of annual emissions reporting under SARA Title III has resulted in quantification of facility-specific environmental release information that may not have otherwise been developed. As a result industry management has the opportunity to evaluate resultant off-site environmental exposure to facility releases where a major focus is frequently on toxic air pollutants. Among the variety of reasons that a company may wish to assess the ambient impact of reported SARA (and other quantified) emissions are:

- Investigate/remediate a known or perceived exposure problem
- Evaluate compliance with existing or anticipated state air toxics program requirements
- Design and manage air emission reduction program to maximize effectiveness in terms of risk reduction
- Anticipate and allay public concerns regarding potential health risks.

As opposed to criteria pollutants, air toxics emissions at an industrial manufacturing facility are often characterized by a number of chemicals from a variety of source types (e.g., stacks, surface vents, fugitive leaks) scattered throughout a plant. The number and type of sources to be addressed results in

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a complex evaluation of off-site impacts. This task becomes even more problematic when attempting to evaluate air toxics impacts on a corporate-wide basis when many disparate facilities located in states with differing air toxics regulations are involved. It is usually necessary in these cases to focus analyses and resources on particular toxic substances, sources, and facilities that pose the greatest impact potential.

Whether screening or refined analysis is conducted, the accuracy of the results depends on the quality of the emissions and source data provided. The level of effort expended on an air impact assessment program should be commensurate with the precision of the emissions characterization for the site and the desired use of the end product. For instance, if only limited emission rate data for an entire site are available then approximate and conservative screening modeling methods may suffice. If, however, screening modeling indicates potentially significant impacts, a more refined analysis of emissions rates, source characteristics and atmospheric dispersions may be warranted.

The analysis procedure described here is designed to provide a consistent basis across different operations and facilities on which to evaluate health risks for all emitted substances. It uses a screening process where the potential for health impacts are first identified and then quantified. The sequence of the analysis steps is illustrated in Fig. 1. The first step in the procedure is to identify appropriate exposure criteria for each substance to be evaluated. This is followed by a series of screening modeling techniques to help identify any substance that has the potential to pose significant risk. The final steps, if necessary, involve a detailed quantitative analysis of impacts including source characterization, refined modeling and, ultimately, risk assessment. Each of these procedures will be described in detail followed by a case study demonstrating the methodology.

Exposure criteria

The intent of establishing exposure criteria at the outset of an air toxic evaluation is to provide a consistent basis for the evaluation of many chemicals in terms of human health effects and to provide continuity among sites. Exposure criteria may account for chronic toxic effects, carcinogenicity or reversible short-term effects. A review of current and proposed state air toxics programs indicates a wide disparity of ambient acceptance criteria in terms of toxicological basis, target risk levels, safety factors and averaging times [1]. While a review of compliance with individual state requirements is appropriate for each facility, this alone may not adequately address all health effects of concern. For instance, limits based on workplace exposure standards may not be sufficiently protective for carcinogenic effects. Although most states are moving toward properly founded (toxicological or epidemiological) air toxics guide-



Fig. 1. Sequence of air toxic assessment steps.

lines and standards, others are limiting program growth in anticipation of federal requirements associated with the Clean Air Act Reauthorization.

In developing exposure criteria to be applied to the air toxics evaluation, we consider measures that are based on sound science yet are sufficiently conservative to eliminate most substances that do not result in adverse off-site impacts. In lieu of establishing specific health effects acceptance criteria, we introduce the concept of an "Ambient Benchmark Level" which can be used as an evaluation measure to rank impacts in terms of potential toxic effects. Excursion above a benchmark does not necessarily indicate that an impact poses unacceptable risk. Rather, comparison of modeled impacts to benchmarks would result in one of two outcomes: (1) lower than benchmark—an indication that adverse health impacts are very unlikely such that further analysis is probably not warranted; (2) higher than benchmark—an indication that a more refined analysis in terms of emissions quantification, modeling or risk assessment is appropriate to determine actual risk, if any.

The evaluation and selection of benchmarks would best be performed by a specialist in environmental health or toxicology. A listing of available criteria is provided in Table 1. Benchmark values for chronic toxic effects can be based on existing health effects criteria such as U.S. EPA Reference Air Concentrations. Some state ambient guidelines or standards have undergone extensive toxicological review and, thus these may also be appropriate. Workplace exposure limits, with an adjustment factor to account for occupational versus community exposures may be most appropriate for short-term irritational effects especially if ambient guidelines are not available.

For carcinogens cancer potency factors developed by the U.S. EPA Carcinogen Assessment Group may be used. A benchmark can be developed by equat-

Criteria	Units	Source	<u></u>
Non-carcinogens			
Reference air concentration	$\mu g/m^3$	U.S. EPA [2]	
Reference dose ^a	mg/kg-day	U.S. EPA [3]	
Acceptable ambient limits	$\mu g/m^3$	State programs	
		(STAPPA, [4])	
Carcinogens			
Unit risk factor	$(\mu g/m^3)^{-1}$	U.S. EPA [2]	
Potency slope ^b	$(mg/kg-day)^{-1}$	U.S. EPA [3]	
Acceptable ambient limits	$\mu g/m^3$	State programs	
based on 10^{-5} to 10^{-6}		(STAPPA, [4])	
target risk		•	
Workplace exposure			
Threshold limit value	mg/m ³	ACGIH [5]	
Permissible exposure limits	mg/m^3	OSHA [6]	
Recommended standards	mg/m^3	NIOSH [6]	

TABLE 1

Available exposure criteria for benchmark development

^aConverted to an air concentration by U.S. EPA assuming a 70 kg body weight and 20 m³/day inhalation rate.

^bTypically converted to a unit risk factor by U.S. EPA by assuming a 70 kg body weight and 20 m^3 /day inhalation rate.

ing exposure to a selected risk level. Commonly applied targets for incremental individual lifetime cancer risk levels fall in the range of one chance in 100,000 to one chance in 1,000,000.

State air toxics programs review impacts for a wide variety of averaging times ranging from 15-minutes, 1-hour, 8-hours, 24-hours to annual average. To simplify the air toxics evaluation process we suggest one or two benchmarks be selected for each substance; an annual benchmark to evaluate chronic and carcinogenic effects and/or 1-hour benchmark for short-term or irritational effects.

Air quality screening approach

When dealing with multiple substances, sources and facilities, it is advantageous to have a standardized modeling procedure in place. To conserve time and resources it may not be necessary to precisely quantify off-site impacts for all substances, but rather to first identify substances that pose negligible offsite risk and, therefore, do not need to undergo a refined assessment. This can be accomplished through an efficient screening procedure.

Level I screening procedure

Level I screening applies simple conversion factors which relate short and long-term emissions to "absolute worst-case" ambient concentrations. A conversion factor appropriate for a peak 1-hour concentration is used in conjunction with maximum short-term emission data for substances with 1-hour benchmarks. For substances with annual benchmarks a long-term conversion factor is applied.

The Level I screening factors can be developed by implementing the U.S. EPA SCREEN model with unit emissions and worst case source/receptor and building configurations appropriate for the particular types of emission sources and facilities to be evaluated. Typical modeling parameters with default (worst-case) values are provided in Table 2. The EPA SCREEN model accounts for building wake and cavity effects and differences in rural and urban turbulent dispersion. Applying the combination of the lowest source height, shortest distance to fenceline and highest building that would be encountered will normally result in a Level I conversion factor representing the minimum amount of dilution (i.e., maximum concentration) that would be expected.

The EPA SCREEN model predicts a maximum 1-hour concentration. Maximum predicted annual average concentrations in the vicinity of industrial facilities are often one to five percent of the predicted peak 1 hour concentration. Therefore, for Level I screening it may be appropriate to conservatively estimate the annual concentration to be 10 percent of the 1-hour factor. Because it is assumed in Level I screening that facility-wide emissions are released at a single location, the results represent upper bound estimates of ambient concentrations.

TABLE 2

Input data requirements for screening modeling

Source data		Typical Level I default value	
Poin	t source		
$Q_{\scriptscriptstyle \mathrm{D}}$	Maximum or annual average emission rate (g/s)	None	
Ń	Distance to fenceline (m)	10	
$H_{ m s}$	Stack or release height above ground (m)	5	
V	Vertical exit velocity (m/s)	0	
Τ	Exit temperature (K)	Ambient	
R	Stack diameter (m)	0.1	
H_{b}	Height of tallest building within 5 $H_{\rm b}$ of source (m)	5	
Area	source		
QA	Maximum or annual average emission rate (g/s)	None	
\boldsymbol{S}	Dimensions of a square area source (m)	5	
$X_{\rm A}$	Distance from edge of area to fenceline (m)	10	
Z_*	Release height (m)	0	

Level II screening procedure

If application of the Level I emissions-to-concentration scaling factor results in a predicted off-site concentration exceeding the benchmark established for the particular substance, then the next step is to perform more detailed ambient screening using site and source-specific data. In Level II screening, we replace the worst-case Level I parameters in Table 1 with actual values for each source. The maximum off-site concentration is predicted for each source using EPA SCREEN. The maximum concentration for all contributing sources are summed to obtain an estimate of total facility impact. The result is still conservative because the off-site location of maximum impact is likely to differ among sources whereas the analysis assumes that the maximum impacts are additive.

For sites with many similar point sources it may be laborious to screen each source independently. In such cases sources can often be grouped to help simplify the analysis. Emissions inventories developed for SARA Title III also often involve substantial emissions from non-point sources such as emissions from building ventilation, tank farms and loading operations. These types of sources, as well as groups comprised of many non-buoyant point sources, can be modeled as area sources with the SCREEN model.

Refined modeling

When a Level II screening analysis indicates that ambient concentrations may exceed the benchmark, a refined analysis may be appropriate. Typically, refined modeling may result in a decrease in concentrations by up to an order of magnitude from the Level II screening results.

Refined modeling involves the application of appropriate U.S. EPA models such as the Industrial Source Complex (ISC) model. The ISC model can account for the precise source configuration, the effects of building wakes as a function of wind direction, meteorological conditions representative of the area, fenceline and other off-site locations and variable terrain elevations. Unlike the SCREEN model the application of ISC (as well as other refined modeling techniques) requires a substantial degree of expertise. Most detailed applications will need to be performed by specialists who keep abreast of the latest model developments and guidance and have experience with these types of applications in a regulatory compliance context.

Two versions of ISC are applicable depending on whether 1-hour or annual concentrations are of most interest. To predict peak 1-hour impacts, ISC-Short Term is implemented using sequential meteorological data consisting of an hourby-hour record of surface wind speed wind direction, turbulence stability class and boundary layer mixing height. Representative meteorological data is often available from a local National Weather Service (NWS) station as reported to the National Climatic Center. Meteorological data are also sometimes available from on-site or other nearby monitors. The use of representative meteorological data is especially important in areas influenced by geographical features such as valleys, shorelines and terrain. For cases where annual concentrations are of most interest, ISC-Long Term can be applied using meteorological data in the form of a climatological frequency distribution of wind direction, wind speed and stability class.

Results from ISC are provided at discrete model receptor locations identified by the user. Receptors are normally placed along the fenceline or plant boundary and beyond to distances where air quality impacts are expected to be insignificant. The results of the Level II screening analysis can be helpful in identifying proper receptor locations. In addition off-site locations of special interest such as schools and hospitals are often included in the model receptor grid. Results from the ISC short-term model can be developed for averaging periods ranging from an hour to a year. In addition to the several highest concentrations that occur at each receptor, model results can be statistically processed to evaluate the frequency distribution of concentrations of various averaging times. Results can also be plotted on base maps by use of computer graphing techniques to show the spatial distribution of the predicted concentrations. This method of displaying results is especially useful in comparing impacts at various locations.

Risk assessment

After refined modeling, the final step in the evaluation of SARA Title III emission impacts is human health risk assessment. The modeling and analysis procedures followed to this point are aimed at determining whether the selected ambient benchmark is exceeded at any off-site location. However, even if screening or refined-model impacts exceed a benchmark, this does not necessarily indicate that an off-site health hazard exists. A risk assessment is undertaken to evaluate the extent, if any, to which potential and actual exposure may cause health effects.

The National Research Council (NRC), has published recommendations regarding methodologies to conduct health risk assessments [7]. These recommendations have been adopted by U.S. EPA and other regulatory agencies. In accordance with NRC recommendations, the health risk assessment for a facility is comprised of the following four basic steps.

- (1) Hazard identification—Determination of the nature and amount of toxic chemicals potentially released from the facility. Identification of the potential adverse health effects associated with these chemicals.
- (2) Dose-response assessment—Determination of the relation between magnitude of exposure and the potential for specific health outcomes for each pollutant.
- (3) *Exposure assessment*—Determination of the extent of potential human exposure to pollutants emitted into the air by the facility.
- (4) Risk characterization—Description of the nature, magnitude and uncertainty of the health risks associated with each pollutant individually and all of the identified SARA Title III substances collectively.

Each risk assessment will focus on the specific relevant issues that help to reduce the level of uncertainty in the evaluation. The dose-response assessment involves an independent interpretation of available toxicological and epidemiological data. For instance, the published U.S. EPA unit risk factor for a particular carcinogen may reflect an overly conservative interpretation of laboratory studies such that risks are overstated. The exposure assessment may differentiate between the hypothetical "maximum individual" who lives on the fenceline and potentially exposed population. The risk characterization defines whether or not an adverse health risk exists and the level of certainty associated with study findings.

The exposure assessment, in addition to inhalation, may involve the tracking of the deposition of persistent substances and transport through the food chain. In general, volatile substances, once emitted tend to remain airborne and, therefore, result in potential exposure primarily through inhalation. However, emitted substances which are either particulate-bound, aerosol or soluble may more readily be deposited to surface vegetation, soil and water bodies. Some deposited pollutants bio-accumulate through the food chain and ultimately result in greater potential exposure than through inhalation alone. An illustration of direct and indirect exposure pathways is provided in Fig. 2.

At the completion of the risk assessment, a strategy can be formulated to target any significant risks associated with site emissions. Typical actions in-



Fig. 2. Potential direct and indirect human exposure pathways.

clude source reduction, emissions controls, enhanced dispersion through stack optimization and enlarging site boundaries.

Case study application

To demonstrate the procedure, a step-wise air toxics modeling assessment is described for a manufacturing facility emitting several volatile organic compounds (VOC). The number of sources and total annual emissions are listed in Table 3. Sources which range in height from 5 to 30 meters represent incinerators, boilers, and vented fugitive releases. Because all emissions are lowlevel and subject to aerodynamic downwash, the maximum off-site impact is expected to be close to the facility fenceline. For purposes of this case study we will focus on annual average impacts only.

The first step is to identify appropriate ambient benchmark levels for each substance. Because none of these VOC have displayed evidence of carcinogenicity, benchmarks were set in accordance with U.S. EPA Reference dose (Rfd)

TABLE 3

Case study chemical emissions

Chemical	Number of sources	Annual emissions (tons)		
Acetone	30	350		
Methyl cellosolve	5	20		
Methyl ethyl ketone	20	350		
Methanol	20	50		
Toluene	25	230		

-LT

[2] information. To convert to units of air concentration $(\mu g/m^3)$ from the *Rfd* (mg per kg body weight per day), the following factors were applied:

$$Rfd\left(\frac{\mathrm{mg}}{\mathrm{kg-day}}\right) \times \frac{70 \mathrm{kg \ body \ weight}}{20 \mathrm{m}^3 \mathrm{inhaled/day}} \times \frac{1000 \ \mu \mathrm{g}}{\mathrm{mg}} = Rfd \times 3500 \ (\mu \mathrm{g/m}^3)$$

This conversion makes standard assumptions applied by EPA in Health Assessment Documents for toxic gases.

The second step is to conduct simplified Level I screening, assuming that all substances are emitted from a common "worst-case" location. As shown in Table 4 the Level I screening results in worst-case projected annual concentrations exceeded benchmarks for three of the five substances.

A Level II screening assessment for the three identified substances involved grouping emissions into a total of ten sources. As shown in Table 4, this use of more realistic source data resulted in elimination of acetone from consideration, but the Level II results indicated that methyl cellosolve and methyl ethyl ketone (2-butanone) would require a refined modeling assessment.

The ISC-Long Term model was used to simulate emissions from each of the 5 methyl cellosolve and 20 methyl ethyl ketone sources. Receptors were placed along the plant boundary out to a distance of 1 km in each direction using a radial grid. A climatological frequency distribution, based on 5 years of National Weather Service weather observations at a nearby airport, were used in ISC. A wind rose, a graphical representation of this distribution, is shown in Fig. 3. The wind rose indicates that emissions are transported most often toward the southeast and north, such that the highest annual concentrations are expected in these directions. The results of the refined ISC modeling (Table 2) indicate only methyl cellosolve has impacts exceeding the benchmark.

The plot of the modeled annual concentrations for methyl cellosolve is provided in Fig. 4. As expected based on the wind rose, highest concentrations extend to the north and south with the lowest concentrations to the west. The

TABLE 4

Chemical	Benchmark ^a	Predicted concentrations			
		Level I	Level II	ISC	
Acetone	360	580	215	NA	
Methyl cellosolve	10.5	33	23	12	
Methyl ethyl ketone	315	580	362	110	
Methanol	1750	83	NA	NA	
Toluene	3500	380	NA	NA	

Case study annual average impacts ($\mu g/m^3$)

^aBenchmarks based on U.S. EPA Reference Dose.

NA-Not applicable where previous step modeling indicated impacts less than benchmark.





maximum concentration occurs at the location denoted by a star in the figure. Predicted concentrations exceeding the benchmark are isolated along the southeastern plant boundary.

One aspect of a risk assessment is to examine potential off-site exposure locations. Shaded areas of the plot indicate residential areas where the potential for long-term exposure is greatest. The central area running parallel to the railway is a commercial industrial zone where long-term (24 h/day, 35 days/ year) exposure is much less likely. The plot indicates that the highest concentration in residential areas is only about 20% of the ambient benchmark. The maximum time a typical individual is likely to occupy a commercial/industrial area is about 40 h/week. Therefore, the maximum long-term off-site exposure concentration associated with facility emissions is only about one-fourth of what would be indicated by the predicted 12 μ g/m³ concentration. This results in an equivalent long-term exposure concentration of 3 μ g/m³, about 30% of the benchmark value. As the exposure analysis alone was able to demonstrate



Fig. 4. Hypothetical annual methyl cellosolve concentration distribution for the case study (units are tenths of the benchmark value).

that the benchmark is effectively not exceeded, other aspects of the risk assessment (e.g., dose-response effect, risk characterization) were not pursued for this case study.

Summary

The ambient air toxics review procedure described herein is designed to provide guidance in optimizing emission reductions to obtain the most benefit in terms of off-site impacts. The procedure involves a stepwise process:

- Emissions estimation
- Setting ambient benchmark levels
- Level I plant-wide emissions screening
- Level II source-specific screening
- Refined modeling
- Risk assessment

Screening procedures can quickly identify the sources and substances to be targeted for control or further evaluation. Refined modeling and risk assessment can then provide a more definitive understanding of potential impacts and their consequences.

References

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