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Off-site toxic consequence assessment: A simplified modeling procedure and case study

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Abstract

An assessment of off-site exposure from spills/releases of toxic chemicals can be conducted by compiling site-specific operational, geographic, demographic, and meteorological data and by using screening-level public-domain modeling tools (e.g., RMP*Comp, ALOHA and DEGADIS). In general, the analysis is confined to the following: event-based simulations (allow for the use of known, constant, atmospheric conditions), known receptor distances (on the order of miles or less), short time scale for the distances considered (order of 10's of minutes or less), gently sloping rough terrain, dense and neutrally buoyant gas dispersion, known chemical inventory and infrastructure (used to define source-term), and known toxic endpoint (defines significance). While screening-level models are relatively simple to use, care must be taken to ensure that the results are meaningful. This approach allows one to assess risk from catastrophic release (e.g., via terrorism), or plausible release scenarios (related to standard operating procedures and industry standards). In addition, given receptor distance and toxic endpoint, the model can be used to predict the critical spill volume to realize significant off-site risk. This information can then be used to assess site storage and operation parameters and to determine the most economical and effective risk reduction measures to be applied.

Keywords: RMP*Comp; ALOHA; DEDADIS; Consequence; Dispersion

1. Introduction

Given heightened public awareness of chemical plant safety issues from media coverage of catastrophic accidents and the threat of terrorist attacks, off-site consequence risk analysis from releases of toxic chemicals has taken on new meaning. Not only must the analysis provide a technical basis for risk portfolio development (assess risk reduction measures in place for "plausible" releases), but also it must provide a component for public relations management with respect to perceived risk. For example, accurate reporting for EPA's risk management program (RMP) is not only required for regulatory compliance, but it is important for public relations because some of the information is in the public record.

This paper presents a simplified, yet useful, procedure for assessing off-site risk exposure from spills/releases of toxic chemicals that includes compilation of site-specific operational, geographic, demographic, and meteorological data and the use of public-domain computer modeling tools. This approach allows one to assess risk from catastrophic release (e.g., via terrorism), or plausible release scenarios (related to standard operating procedures and industry standards). In addition, given receptor distance and toxic endpoint (TE), the procedure can be used to predict the critical spill volume necessary to realize significant off-site risk as a function of meteorology. This information can then be used to assess site storage and operation parameters and to determine the most economical and effective risk reduction measures to be applied.

2. Approach

To develop modeling tools and procedures that meet the objectives for off-site consequence analysis (OCA) set forth above, the approach must consider the following components. First the fundamental physical problem attributes and parame-

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ters must be defined. In general, the analysis is confined to the following:

- Event-based simulations. This attribute allows for the use of known, constant, atmospheric conditions.
- Known receptor distances, ranging from 100 s of yards to several miles. For example, the distance to the facility's fenceline or the nearest road or school.
- Short time scale for the distances considered, ranging from seconds to 10's of minutes depending on wind speed and the proximity of the receptor to the spill.
- Flat to gently sloping rough terrain. This is a typical condition associated with industrial facility siting.
- Dense to neutrally buoyant gas dispersion. Many toxic compounds are emitted as dense vapor clouds which disperse over distance to form neutrally buoyant plumes.
- Known chemical inventory and handling infrastructure. This is used in part to define the source-term, i.e., storage volumes, loading and unloading procedures, passive mitigation measures in place (e.g., diking), and administrative controls in place (e.g., automatic valve shutoff, foaming, etc.).
- Known TE. This is the concentration and exposure time that defines significance for adverse human impact.

Given these problem attributes, the second component is to identify applicable models that represent the state-of-the science and that have utility at the site-level. By utility we mean that the models can describe the physical problem as defined above, that they are accepted by the regulatory and industrial communities, and that they are well documented for model use and capability understanding. In addition, utility also relates to model complexity in terms of data needs and level of expertise required to run the model. The class of models capable of simulating the problem described above is considered to be "screening" because they use various simplifying assumptions to minimize parameter input while providing the essential problem physics.

A review of EPA's guidance for off-site consequence analysis [1] identified a series of complementary public-domain screen-

Table 1
Comparison of complementary models capable of simulating a wide range of toxic release scenarios

Model	Attributes
RMP*Comp	Simple screening model (meant to give conservative results) Generalized table lookup User-friendly interface Minimal parameter input Easy to use, no modeling experience required Tables generated from ALOHA (neutrally buoyant) and SLAB (dense gas) Averaging time: 10 min for 10 min release, 30 min for 60 min release Simple (conservative) emissions model Fixed chemical library
ALOHA	Screening model (refined relative to RMP*Comp) User-friendly interface Basic understanding of air dispersion parameters required. Well documented for model utility. Neutrally buoyant (plume and puff) and dense gas dispersion algorithms Computes ground-level concentrations as a function of time Elevated release only for neutrally buoyant releases, else ground-level release. Time scale: 1 min to 1 h Applicable space-scale >100 m and <10 km Extensive, editable, chemical library Additional input for source and meteorology Ground roughness: dense gas: 1 cm $\leq$ length $\leq$10 cm; neutral gas: length = 3 cm if rural, = 100 cm if urban Dispersion averaging time: adjusted to 5 min A simplified version of DEGADIS (predictions avg.% 110 of DEGADIS) Sophisticated emissions model (considers transient source-term) Internal source types: direct (gas), puddle (liquid), tank release (gas and liquid) and pipe release (gas) Externally computed source rate incorporated through direct source condition (point source)
DEGADIS	Used when technical accuracy required (refined relative to ALOHA) No interface available No internal emissions model Time-variable source evolution rate defined from external model Generic source configuration (elevated/ground, jet/area) User-specified averaging time (empirical scaling of inherent 10 min averaging time) Dispersion of chemical mixtures through conservation of contaminant mole fraction (for the nonaerosol case) Dispersion of an initial pure contaminant aerosol through isothermal mode (user-specified concentration—density relationship) Computes ground-level or elevated concentrations as a function of time Applicable space-scale >100 m and <10 km Difficult to use, experience in fluid dynamics and atmospheric science required.

Model complexity increasing from top to bottom.

ing modeling tools: RMP*Comp, ALOHA and DEGADIS, that when used in concert, provide a diverse toolbox that meets the requirements for site utility. The use of a particular dispersion model is dictated by chemical composition and release conditions. The attributes for these models are summarized in Table 1. Upon review of Table 1, one should note that the models are complementary in terms of complexity and model basis. Specifically, RMP*Comp can be considered a simplified version of ALOHA, and ALOHA can be considered a simplified version of DEGADIS (discussed further below). The reason for using a complementary set of models is threefold:

- It allows one to incorporate additional problem complexity when the need exists and the data are available.
- It allows for a form of model verification, by comparing independent model results (i.e., models with the same theoretical underpinnings should provide similar results).
- It allows one to refine the model result on an as-need basis, where in general more accurate screening results are obtained as model complexity (and data needs) increases.

RMP*Comp is a simplified screening tool; it is set up to be fast and easy to use and it has minimal input requirements. Its predictions are necessarily conservative to offset uncertainty associated with simplifying assumptions. RMP*Comp is an automated version of the EPA's off-site consequence analysis guidance. Model documentation is available on the Internet [2].

ALOHA (areal locations of hazardous atmospheres) is a computer program that uses site-specific information provided by its user and physical property data from its extensive (and editable) chemical library to predict how a hazardous gas cloud disperses in the atmosphere after an accidental chemical release. The additional data required by ALOHA versus RMP*Comp is not extensive, and the accuracy of the predictions is significantly improved. Although ALOHA makes many approximations over its parent program DEGADIS in order to produce results quickly, its predictions have been checked against estimates made by similar models and measurements made during field experiments to ensure that results are as accurate as possible (documented validity). While ALOHA requires users to have some understanding of the basic parameters associated with atmospheric science, all necessary information on model use and limitations is provided in its self-contained documentation. The ALOHA model (V 5.3.1) and documentation are available on the Internet [3]. In addition, the US Department of Energy has issued a report on ALOHA identifying applicable regimes in accident analysis, default inputs, and special conditions for using the code [4].

Note, the EPA supports a comprehensive computer application called CAMEO, which contains the most recent versions of both RMP*Comp and ALOHA [5].

Finally, as indicated in Table 1, ALOHA is a simplified version of its parent program DEGADIS (dense gas dispersion). The DEGADIS model was originally developed for the US Coast Guard and the Gas Research Institute and subsequent work sponsored by the EPA extended DEGADIS for simulation of the dispersion of vertical jets. Table 1 provides a summary of model capabilities. While DEGADIS is the most comprehensive model of the three listed, it requires experience in fluid dynamics and atmospheric science and a significant amount of additional data to define fluid properties and dispersion parameters, and it has no graphical user interface. Basic information concerning the theoretical development of DEGADIS v2.1, its applicability, and its general implementation are available on the Internet [6].

Table 1 focuses on model capabilities. Equally important are model limitations. This family of models does not account for the following processes:

- Terrain steering effects.
- Chemical reactions.
- Buoyant plume dispersion.
- Particulate wet and dry deposition.
- Dispersion effects caused by building wakes.

While one or more of these processes may come into play for any given problem, engineering judgment can be used to assess the significance of the process on the source and dispersion predictions. For example, omitting buoyant plume dispersion, particulate deposition and building wake effects will yield conservative results (i.e., tend to over-predict impact because these processes tend to add dispersion to plume fate).

3. Model comparison

As discussed above, two reasons to use different models to solve the same problem are model verification and model refinement. To illustrate this point, consider the modeling results shown in Figs. 1 and 2, which are EPA RMP Rule worst case scenario calculations for two regulated compounds at an active chemical production facility. Fig. 1 shows the model-predicted distance to the TE for an allyl alcohol liquid spill. The problem was modeled using each of the three models shown, and model input parameters are provided in Table 2. Fig. 1 shows that while ALOHA and DEGADIS effectively provide the same result,

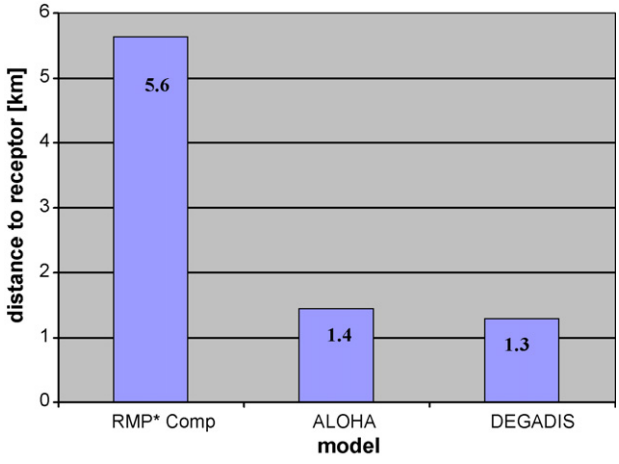

Fig. 1. For a worst case allyl chloride liquid spill as per the requirements of the RMP Rule for OCA. For each model, shows the distance to the TE (15 ppm). Table 2 provides model input parameters.

Table 2
Model input parameters for the results shown in Fig. 1

I/O category	RMP*Comp (V 1.07)	ALOHA (V 5.3.1)	DEGADIS (V 2.1)
Chemical	Internal library TE = 15 ppm	Internal library TE = 15 ppm	From ALOHA TE = 15 ppm
Dispersion model	Dense gas	Dense gas	Dense gas
Atmospheric conditions	Worst case Urban surroundings	Wind speed = 1.5 m/s at 10 m Surface (Zo) = 10 cm Clear sky, nighttime F stability Temp. = 38 °C	Wind speed = 1.5 m/s at 10 m Surface (Zo) = 10 cm Avg. time = 5 min F stability Temp. = 38 °C
Source conditions	Mass spilled = 82,000 kg Release temp = 38 °C Diked area = 873 m^2 Emission time = 60 min Computed emission rate = 60 kg/min (output)	Type = liquid puddle Mass spilled = 82,000 kg Diked area = 873 m^2 Emission time = 60 min Release temp = 38 °C Computed emission rate = 21 kg/min (output)	Area = 873 m^2 Emission rate = 21 kg/min Emission time = 60 min

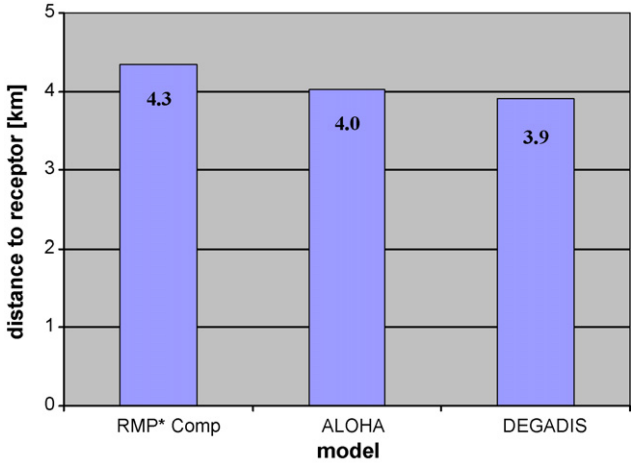

Fig. 2. For a worst case methyl chloride gas release as per the requirements of the RMP Rule for OCA. Table 3 provides model input parameters.

the result from RMP*Comp shows three times the impact distance. The major reason for this discrepancy can be traced to the source emission rate used in each model. ALOHA's internal puddle emissions model was used to compute the emission rate for both the ALOHA and DEGADIS result (Table 2). RMP*Comp's internal emissions model was used to compute its emission rate (Table 2). Upon reviewing the documentation for each model [2,3], RMP*Comp's emissions model is a simpler, more conservative, approximation of that used in ALOHA.

Fig. 2 shows the model-predicted distance to the TE for a methyl chloride gas release. Table 3 provides model input parameters for the three models considered. Fig. 2 shows that all three models provide qualitatively the same result, where in this case all three models use the same source-term.

This simple analysis shows that an accurate source emission rate estimate is an important component for OCA. It illustrates that a significant reduction in impact distances is normally predicted by dispersion modeling programs that include higher degree of incorporated physics and commensurately require more specific input data (more data leads to less uncertainty and greater accuracy). In addition, it appears that, in general, the ALOHA model provides the highest degree of site utility due to its ease of use (graphical user interface and extensive documentation) and its emissions estimation capabilities (Table 1). RMP*Comp may be used as a verification check, and DEGADIS should be used on an as-need basis when the physics of the problem dictates.

Table 3
Model input parameters for the results shown in Fig. 2

I/O category	RMP*Comp (V 1.07)	ALOHA (V 5.3.1)	DEGADIS (V 2.1)
Chemical	Internal library TE = 400 ppm	Internal library TE = 400 ppm	From ALOHA TE = 400 ppm
Dispersion model	Dense gas	Dense gas	Dense gas
Atmospheric conditions	Worst case Urban surroundings	Wind speed = 1.5 m/s at 3 m Surface (Zo) = 10 cm Clear sky, nighttime F stability Temp. = 38 °C	Wind speed = 1.5 m/s at 3 m Surface (Zo) = 10 cm Avg. time = 3 min F stability Temp. = 38 °C
Source conditions	Mass released = 155,000 kg Emission rate = 15,500 kg/min Emission time = 10 min	Type = direct Emission rate = 15,500 kg/min emission time = 10 min	Source radius = 0.1 m Emission rate = 15,500 kg/min Emission time = 10 min

4. Application

To illustrate the modeling approach for off-site consequence risk analysis, consider the following case study from an active chemical production facility. The goal for the study was to evaluate if the existing risk reduction measures are sufficient to prevent spills of highly toxic chemicals in quantities that would create a significant off-site impact.

The procedure for meeting the objectives is to apply the following systematic approach.

4.1. Define significant off-site consequence

Significant off-site consequence is defined through the use of the toxic endpoint (TE), which provides the time interval and level (concentration) of exposure. For this study, the following TE definitions were used:

- Instantaneous exposure to IDLH concentrations.
- Sustained ($\geq$30 min) exposure to ERPG-2 concentrations.

These are conservative applications of these thresholds to account for uncertainty in model predictions, and both parameters are used to assess different levels of risk.

4.2. Define receptor distance

The distance to the nearest off-site receptor is that from the spill site to nearest point where off-site human involvement is likely to occur. For example, this is as close as the fence-line or as far as the nearest school, building or road. For this case study, the nearest receptor was defined as a major highway 0.8 km from the spill site.

4.3. Identify chemicals of concern (COC)

COCs are those highly toxic chemicals that if released in sufficient quantity have the potential for off-site consequence.

- List all relevant compounds. Include raw materials and intermediate and finished products. Use RMP guidance, site and industry standards, and engineering judgment. For the case study the following COCs were identified: allyl alcohol, methyl chloride, and boron trifluoride.
- For each compound identified, compile the following attributes that assist in defining the emission source-term and off-site impact:
  - Toxic endpoint, i.e., IDLH and ERPG-2 concentrations.
  - Material properties (e.g., molecular weight, heat capacity, vapor pressure, density, heat of combustion, etc.).
  - Physical state (liquid or gas).
  - Amount delivered and stored onsite.
  - Passive mitigation measures in place (e.g., diking to contain liquid spills, pipe diameters constraining gas flow, size of storage vessel, etc.).

Note that ALOHA's internal chemical database includes the physical properties for many compounds, and it can be edited to include other compounds of interest.

4.4. Define methods and assumptions used to quantify off-site toxic impact

The approach is to use air-modeling analysis to determine, for each COC, the amount of material that needs to be spilled in order to have significant off-site consequence at the receptor under the following meteorological conditions:

- Worst case: low wind speed (1.5 m/s), very stable atmosphere (class F) and highest recorded site-specific temperature.[1] This is defined as relatively low probability occurrence.
- Alternative case: average atmospheric conditions obtained from site-specific metrological data. For the case study we have data from the nearest airport: D stability, 4.1 m/s wind speed and 19.4 °C. This is defined as a higher probability occurrence.

The reason for choosing two atmospheric conditions is to provide information on parameter sensitivity (emission rate and dispersion) and to account for model uncertainty in quantifying risk.

For this case study, the maximum release volume was limited by the following worst case scenario: the release of the largest quantity from a single vessel or process line failure. Liquid spills are modeled as puddles of constant depth constrained in area by the current diking associated with the various areas associated with storage and handling (an existing passive mitigation measures). Gas emissions are modeled as releases from a circular tank opening (e.g., open valve or pipe of known diameter).

The results from the case study using the ALOHA model are presented in Tables 4–6, for allyl alcohol, methyl chloride and boron trifluoride, respectively. For an allyl alcohol liquid spill ALOHA's puddle evaporation model was used to estimate the emission rate. Table 4 shows that under worst and alternative case meteorology conditions, an uncontrolled liquid spill of 190 and 3200 l, respectively, can result in the ERPG-2 TE at the receptor. In addition, a spill of 3900 l can result in the IDLH TE at the receptor under worst case meteorology. These quantities produce pool areas (a surrogate for source strength) that are far below the passive mitigation measures in place (compare spill area with containment area), indicating that this passive measure alone is insufficient to mitigate risk. Also note that the spill volumes are small enough to render storage vessel size an infeasible passive mitigation measure. Fig. 3 shows the data graphically, where the spill area required to emit sufficient mass to reach the TE at the receptor for each of the four cases is compared to the current diked area (passive mitigation measure in place). It can be seen that the passive mitigation measures in place are only protective against realizing the IDLH TE at the receptor when

[1] Because F stability by definition only occurs at night, the high nighttime temperature should be used.

Table 4
Allyl alcohol liquid spill under worst and plausible case meteorology—'Spill area' indicates the pool size necessary to realize the TE at the receptor (0.8 km away)

Site-defined toxic endpoint	Spill area (m^2)	Containment area (m^2)	Release volume (l)	Release weight (kg)	Storage weight (kg)	Time to receptor (min)
Worst case meteorology[a]						
2 ppm (sustained, >30 min)	19	RC = 873;	190	159	RC = 82,000;	16
IDLH: 20 ppm (instantaneous)	390	ST = 793	3,900	3,266	ST = 50,000	18
Alternative case meteorology[b]						
2 ppm (sustained (>30 min)	320	RC = 873;	3,200	2,700	RC = 82,000;	5
IDLH: 20 ppm (instantaneous)	3200	ST = 793	32,000	27,000	ST = 50,000	5

For comparison, the 'containment area' is the existing passive mitigation (RC = rail car unloading area, ST = storage tank area). Assuming the spill area is 1 cm deep, the 'total release volume' and 'weight' are computed as shown. The 'time to receptor' is the time it takes for the plume to arrive at the receptor.

[a] Meteorology: nighttime, clear sky; wind speed = 1.5 m/s at 10 m; stability = F; air temp. = 38 °C. Surroundings: between urban and rural (Zo = 10 cm); source type: puddle at ambient temp.

[b] Meteorology: daytime, overcast; wind speed = 4.1 min/h at 10 m; stability = D; air temp. = 19.4 °F. Surroundings: between urban and rural (Zo = 10 cm); source type: puddle at ambient temp.

Table 5
Methyl chloride gas release under worst and plausible case meteorology—'Opening diameter' is the tank opening size necessary to allow the 'release rate' that is necessary to realize the TE concentration at the receptor (0.8 km away)

Site-defined toxic endpoint	Opening diameter (cm)	Transfer line diameter (cm)	Release rate (kg/min)	Release duration (min)	Total released (kg)	Storage weight (kg)	Time to receptor (min)
Worst case meteorology[a]							
ERPG-2: 400 ppm (sustained, >30 min)	<5.1	5.1	590	35	20,639	RC = 82,000,	14
IDLH: 2000 ppm (instantaneous)	10.2		3175	5	15,876	ST = 155,000	15
Alternative case meteorology[b]							
ERPG-2: 400 ppm (sustained, >30 min)	6.4	5.1	1100	33	36,300	RC = 82,000,	5
IDLH: 2000 ppm (instantaneous)	16.5		8100	3	24,300	ST = 155,000	5

The release must last for the 'release time' for the TE to be realized at the receptor. The 'total released' is based on the release rate and time. The 'time to receptor' is the time it takes for the plume to arrive at the receptor.

[a] Meteorology: nighttime, clear sky; wind speed = 1.5 m/s at 3 m; stability = F; air temp. = 38 °C. Surroundings: between urban and rural (Zo = 10 cm); source type: direct, constant rate; relate tank opening diameter to emission rate using ALOHA tank model (see Fig. 4 for model input).

[b] Meteorology: daytime; overcast; wind speed = 4.1 m/s at 10 m; stability = D; air temp. = 19.4 °C. Surroundings: between urban and rural (Zo = 10 cm); source type: direct, constant rate; relate tank opening diameter to emission rate using ALOHA tank model (see Fig. 4 for model input).

alternative meteorology conditions prevail. Finally, referencing Table 4, the modeling analysis provides an estimate of problem time-scale (last column). Specifically, depending on wind speed, significant concentrations at the receptor can occur in as little as 5 min. This provides insight into potential administrative and emergency response measures.

Table 5 provides the modeling analysis for a methyl chloride gas release. In this case methyl chloride is assumed to be released as a gas from a storage tank containing 155,000 kg through a circular opening (valve or pipe). ALOHA's tank release model was used to estimate the emission rate as a function of opening diameter, where the tank opening constrains the rate of release. The table shows the tank openings and release times necessary to realize the TE and the time it takes for the vapor cloud to arrive at the receptor for the two meteorological conditions. Fig. 4 provides a graphical display of the model result. Using tank opening as a surrogate for emission rate, the plot shows the computed impact at the receptor (concentration) as a function of tank opening. The data shows that risk for adverse off-site consequence can be nearly eliminated by using 5.08 cm (2 in.) diameter transfer piping (i.e., 2 in. diameter transfer lines are an effective passive mitigation measure).

Table 6
Boron trifluoride gas release under worst case meteorology—the amount stored in a single vessel is shown

Site-defined toxic endpoint	Release rate (kg/min)	Release duration (min)	Total released (kg)	Amt. stored in one container (kg)	Time to receptor (min)
Worst case meteorology					
ERPG-2: 11 ppm (sustained, >30 min)	7.7	33	254	27	11
IDLH: 25 ppm (instantaneous)	34	3	102		11

The 'release rate' and 'release time' are that necessary to realize the TE at the receptor (0.8 km away). The resulting 'total released' is computed, and the time it takes for the plume to reach the receptor is shown. Assuming that a worst case release is the total quantity stored in a single vessel, the data show that the risk for significant off-site consequence is insignificant (i.e., container size is an effective passive mitigation measure). Meteorology: nighttime, clear sky; wind speed = 1.5 m/s at 3 m; stability = F; air temp. = 38 °C. Surroundings: between urban and rural (Zo = 10 cm); source type: direct, constant rate.

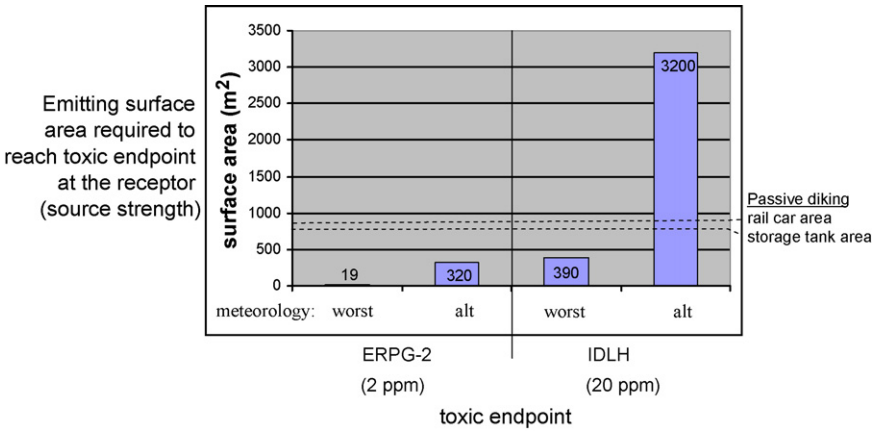

Fig. 3. Allyl alcohol spill—for the data presented in Table 4, using surface area as a surrogate for emission rate, compare the surface area required to emit sufficient mass to reach the TE at the receptor as a function of meteorology. If the bar is below the passive diking line, then the risk is not mitigated.

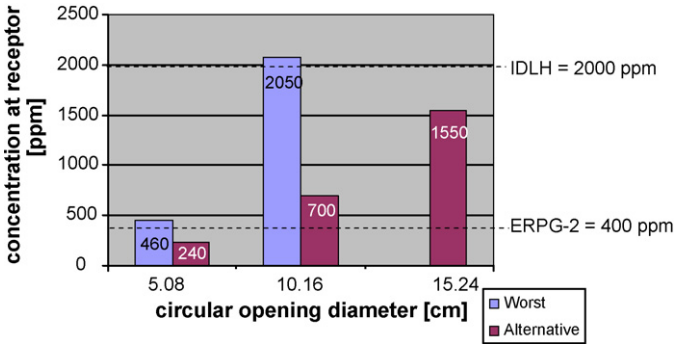

Fig. 4. Methyl chloride release—using tank opening as a surrogate for emission rate, the bars show the computed impact at the receptor (concentration) as a function of tank opening. For reference the TEs are shown. The data show that risk for adverse off-site consequence can be nearly eliminated by using 5.1 cm (2 in.) diameter transfer piping. ALOHA model input: atmospheric conditions as defined in Table 5 for worst and alternative cases, source: type = tank, tank dimensions = 4.57 m diameter, 11 m length, material stored at 25 °C for worst case and ambient temperature for alternative case, opening via pipe/valve at bottom of tank.

Finally, Table 6 provides the model result for a boron trifluoride (B3F) gas release. Assuming that a worst case release is the total quantity stored in a single vessel (27 kg in this case), the data shows that the risk for significant off-site consequence is insignificant (i.e., container size is an effective passive mitigation measure).

4.5. Screen COCs based on the critical release volumes

Based on the modeling exercise described above, only those COCs that pose a plausible risk of realizing significant off-site impact are retained for development of a risk portfolio. For the case study, allyl alcohol and methyl chloride are retained and B3F is eliminated.

The risk portfolio challenges the risk reduction measures in place. In particular, the risk manager asks whether the spill quantities reported in the screening analysis above are plausible, and if so whether the emission control measures in place (passive or administrative) are sufficient to manage the potential risk. Knowing release volumes and process, one can determine the most cost-effective risk reduction measures to be applied.

5. Conclusions

A systematic modeling approach to assess risk of off-site consequence from spills/releases of toxic chemicals was described. The approach takes advantage of the relatively short time- and space-scales associated with accidental chemical releases. As described, screening-level modeling analysis is appropriate for most situations. By comparing models of different levels of complexity it was found that a significant reduction in impact distances is normally predicted by dispersion modeling programs that include a higher degree of incorporated physics and commensurately require more specific input data (more data leads to less uncertainty and greater accuracy). The public-domain model ALOHA was found to have adequate utility at the site-level because it provided a balance between site-specific data needs and ease of use (graphical user interface and extensive documentation), and because it is known and accepted by the regulatory and industrial communities. RMP*Comp was found to be useful as a verification check, and DEGADIS should be used on an as-need basis when the physics of the problem dictates.

The modeling results provide important information for risk analysis:

- Chemicals of concern: which chemicals pose a significant risk?
- Release scale: an indication of release quantity and meteorology conditions required to realize a significant off-site toxic impact.
- Reaction time scale: how long it takes for toxic conditions to be realized at the receptor.
- A technical basis upon which to judge the efficacy of passive mitigation measures (container volume, diking and process line diameter).

In summary, the use of more precise tools for OCA will improve our assessment of off-site impact (severity) of potential gas releases and therefore help in defining necessary measures

required to control the risks. The additional accuracy is also necessary for reports to the regulatory agencies for emergency planning and public relations issues.

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