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Toxic Endpoint Analysis

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Abstract

The purpose of this analysis is to compare the toxic endpoints (e.g., ERPG-2, ERPG-3, AEGL-2 AEGL-3, PAC-2, and PAC-3) at both the 15-minute and the 60-minute release periods against the existing Industrial Facilities Safety Basis (IFSB) Guidance Protocol for classifying facilities at Sandia National Laboratories (SNL). In this analysis, specific toxic chemicals are modeled with exposure limits at 100 meters (m) to understand the impacts on facility hazard classification.

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ACRONYMS and ABBREVIATIONS

AEGL	Acute Emergency Guideline Levels
AIHA	American Industrial Hygiene Association
ALOHA	Areal Locations of Hazardous Atmospheres
amu	Atomic mass unit
˚C	degrees Celsius (temperature)
DOE	Department of Energy
EFCOG	Energy Facility Contractors Group
EPA	Environmental Protection Agency
ERPC	Emergency Response Planning Committee
ERPG	Emergency Response Planning Guideline
g/mol	grams per mole
hr	hour
IFSB	Industrial Facility Safety Basis
KAFB	Kirtland Air Force Base
lbs	pounds
lbs/min	pounds per minute
LOC	Level of Concern
m	meters
m/s	meters per second
mg/m3	milligrams per cubic meter
min	minutes
NAC	National Advisory Committee
NAS	National Academy of Sciences
NRCC	National Research Council Committee
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
OSHA	Occupational Safety and Health Act
PAC	Protective Action Criteria
PHS	Primary Hazard Screening
ppm	parts per million
SCAPA	Subcommittee on Consequence Assessment and Protective Action
SNL	Sandia National Laboratories
SNL/NM	Sandia National Laboratories/ New Mexico
TEEL	Temporary Emergency Exposure Limit

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1. PURPOSE

The purpose of this analysis is to compare the toxic endpoints (e.g., ERPG-2, ERPG-3, AEGL-2 AEGL-3, PAC-2, and PAC-3) at both the 15-minute and the 60-minute release periods against the existing Industrial Facilities Safety Basis (IFSB) Guidance Protocol for classifying facilities at Sandia National Laboratories (SNL).

The Department of Energy (DOE) recommends using the updated PAC values in emergency planning. Due to the lack of current ERPG data, and because PACs 1) are becoming more widely available, and 2) are based upon more precise data, there is increasing interest in how these values compare to the conservative “ERPG-3 at 15 minutes (min)” methodology currently in use. It is important for IFSB to be both conservative and realistic when determining hazard classification to 1) ensure that workers, collocated workers, and the public are safe, and 2) that facilities are efficient and productive in executing their processes and projects.

In this analysis, specific toxic chemicals are modeled with exposure limits at 100 meters (m) to understand the impacts on facility hazard classification. As provided by the SNL Safety Basis Manual (SNL 2008) and PLA-05-03, the ERPG-3 levels are currently established as the exposure guidelines for chemical releases for evaluating facility hazard classification.

2. OVERVIEW OF TOXIC ENDPOINTS

Protective Action Criteria (PACs) are chemical exposure values used for evaluating chemical releases. The PAC values can be used to analyze the severity of the potential impacts to the worker, the collocated worker, and the public.

PAC values are based on the following chemical exposure limit values:

- Acute Exposure Guideline Level (AEGL) values, which are provided by the U.S. Environmental Protection Agency (EPA), and are co-developed by the National Academy of Sciences (NAS) and the National Research Council Committee (NRCC).
- Emergency Response Planning Guideline (ERPG) values, which are developed by the American Industrial Hygiene Association (AIHA).
- Temporary Emergency Exposure Limit (TEELs) values, which are provided by the Subcommittee on Consequence Assessment and Protective Actions (SCAPA), but are developed by the Department of Energy (DOE) Office of Emergency Management (NA-41).

For emergency planning, it is Department of Energy policy to use the PAC values with the following hierarchy:

- Use AEGLs (both final and interim values), if they are available.
- Use ERPG values if AEGLs are not available.
- Use TEEL values if both AEGL and ERPG values are not available.

DOE has approved AEGLs for priority use in emergency planning, because they are assumed to be more accurate than ERPGs and TEELs as a result of testing on more refined data.

PAC values are developed in three different levels (-1, -2, and -3), which are distinguished by varying degrees of severity of the toxic effects on exposed personnel.

3. EXPOSURE LIMITS DEVELOPMENT PROCESS

AEGLs were developed by the National Advisory Committee (NAC) over a 15-year period, from 1996 to October 2011. Each AEGL was developed independently by a team of scientists who assigned priorities to current data from both human and animal studies. AEGLs were developed through a review of primary sources of toxicological information, and each value was individually peer-reviewed. The process was exhaustive, and the guidelines were thoroughly reviewed.

As a result, AEGLs represent the best public exposure guidelines available to date. As part of the previous development process, interim AEGL values were reviewed and established by the National Advisory Committee for AEGLs, then were made available for public comment. Interim AEGLs are available for use during the peer review and publication of final AEGLs by the National Research Council Committee of the National Academy of Sciences.

In November 2011, the AEGL development process was modified. Future development of AEGLs will focus on finalizing interim values through the National Academy of Sciences. As of mid-2015, more than 160 substances have been assigned final AEGLs, and approximately 90 substances have interim AEGLs. The AEGL Program web site (http://www.epa.gov/oppt/aegl/) provides information on both the scientific and the policy work used in developing AEGLs.

The ERPG guidelines are clearly defined, and are based on extensive, current data. The rationale for selecting each value is explained; other pertinent information is also provided for each chemical. Each guideline identifies the substance, its chemical and structural properties, associated animal toxicology data, human experience, existing exposure guidelines, the rationale behind the selected value, and a list of references. ERPGs, like AEGLs, are developed through extensive reviews of human and animal studies, and are based on a weight-of-evidence approach, although AEGLs are assumed to be more accurate. As of mid-2015, approximately 145 chemicals have ERPG guidelines.

[NOTE: The AIHA Emergency Response Planning Committee website provides more information on the development of ERPGs.]

To define limits on a more timely schedule, while maintaining high quality, TEELs are derived from secondary data using a specific standard methodology. The methodology manipulates current data using a peer-reviewed algorithm to establish the TEELs. Data sources are either existing exposure limits designed to prevent adverse effects in humans, or experimentally derived toxicity parameters. TEEL values are approximations of potential values, and are subject to change whenever new, or better, information becomes available. Currently, approximately 3,390 chemicals have TEELs.

[NOTE: *The TEELs Method and Practices Handbook details the specific methods used to derive TEEL values. It also presents background information, sample calculations for how the TEELs are derived, and descriptions of the quality assurance measures used in the TEEL derivation process.]

4. DEFINITIONS: AEGLS, ERPGS, AND TEELS

There are subtle differences between the definitions of the toxic endpoints relevant to the comparison of these values. AEGLs seem to be more accurate, because the values are based on both primary toxicological information and human and animal experiments, and are extensively reviewed before publication. AEGLs and ERPGs differ in the included population, as well as in whether the values are above or below thresholds.

AEGLs represent the threshold exposure limits for the general public. AEGLs are developed for each of the five exposure periods (10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours). DOE guidance is to use the 1-hour AEGL values, because these values are assumed to be the most accurate (SCAPA, Definition of PACs). AEGLs are designed to protect the general population, including sensitive individuals, such as the elderly and children. The three tiers of AEGLs are defined below.

- **AEGL-1** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic, non-sensory effects. However, these effects are not disabling, and are transient and reversible upon cessation of the exposure.
- **AEGL-2** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting, adverse health effects, or an impaired ability to escape.

- **AEGL-3** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening adverse health effects or death.

ERPGs are estimates of concentration bounds for specific chemicals, and are developed for a 1-hour exposure period. It is recognized by the AIHA Emergency Response Planning Committee (and it should be remembered by all those who make use of ERPG values) that human responses do not occur at precise exposure levels, but can occur over a range of concentrations.

The ERPG values derived should not be expected to protect everyone, but should be applicable to most individuals in the general population. In all populations there are hypersensitive individuals who will show adverse responses at exposure concentrations below the levels at which most individuals would typically respond. The ERPG value estimates are based on the available data, which are summarized in the documentation. In cases where data is limited, the uncertainty of these estimates is large. Users of the ERPG values are strongly encouraged to carefully review the documentation before applying these values. The three levels of ERPGs are defined below.

- **ERPG-1** is the maximum air concentration below which it is believed nearly all individuals (excluding sensitive individuals) could be exposed for up to one hour without experiencing any symptoms other than mild transient adverse health effects or perceiving a clearly defined objectionable odor.
- **ERPG-2** is the maximum air concentration below which it is believed nearly all individuals (excluding sensitive individuals) could be exposed for up to one hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action.
- **ERPG-3** is the maximum air concentration below which it is believed nearly all individuals (excluding sensitive individuals) could be exposed for up to one hour without experiencing or developing life-threatening health effects.

TEEL values are temporary and should be used to help protect the public when AEGLs or ERPGs are not available. TEELs are based on a 1-hr exposure period, and should only be used to model chemical releases of short-term durations. TEEL values estimate how nearly all individuals would react to a catastrophic release. TEEL levels are defined as follows:

- **TEEL-1** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience notable discomfort, irritation, or certain asymptomatic, non-sensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.

- **TEEL-2** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience either irreversible or other serious, long-lasting, adverse health effects, or an impaired ability to escape.
- **TEEL-3** is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience life-threatening adverse health effects or death.

5. CONVERTING EXPOSURE VALUES

The exposure limits are generally expressed in parts per million (ppm), but can be converted and expressed in milligrams per cubic meter (mg/m^3). The formulas used to convert ppm to mg/m^3 and mg/m^3 to ppm are shown below.

$$\frac{mg}{m^3} = \frac{ppmV\ x\ MW}{24.04} \qquad ppmV = \frac{mg/m^3 x 24.04}{MW}$$

In this analysis, traditional IFSB ERPG and derived values are converted from mg/m^3 to ppm to remain comparable with the current toxic endpoint values published in SCAPA, which are presented in ppm.

6. SCREENING CHEMICALS

The chemicals chlorine (Cl_2), hydrogen bromide (HBr), boron trichloride (BCl_3), and carbon monoxide (CO) are chosen to be evaluated in this analysis based on their current use in several SNL/NM facilities. As a note, these chemicals have hazardous qualities and are, traditionally, the "classifying toxics." Cl_2, HBr and BCl_3 are highly toxic industrial chemicals; CO is a moderately toxic industrial chemical. More information regarding each chemical is provided below.

Chlorine. In its gaseous state, chlorine (CL_2) has a yellowish-green color. It can also be identified by its distinct, irritating odor. As a gas, chlorine has a molecular weight of approximately 70.9 atomic mass unit (amu), which is heavier than the total molecular weight of air. This means the gas will settle in low-lying areas, and can accumulate in large masses. Chlorine can be fatal if inhaled, and can cause watery eyes/blurred vision and a burning sensation in the eyes, nose, mouth, and even on the skin. It can also cause coughing and wheezing due to fluid gathering in the lungs. Shorter term effects of Cl_2 exposure include dizziness, emotional disturbances, and nausea to the point of vomiting. Chlorine is a strong oxidizer, and while is it not flammable by itself, it has the potential to ignite combustibles and to intensify fire. Chlorine must also be isolated from incompatible and hazardous materials.

Examples of incompatibilities are combustible materials, bases, metals/metal salts, reducing agents, halogens, and all oxidizing materials.

Hydrogen Bromide. Hydrogen bromide (HBr) is a colorless gas with a sharp, irritating odor. As a note, HBr is shipped as a liquefied compressed gas, and is often used in an aqueous solution. HBr has a molecular weight of 80.9 amu, and is classified as a "heavy" gas. Hydrogen bromide can be fatal to personnel upon inhalation or exposure. It can also impair eyesight, irritate the nose and throat, and cause skin burns. Hydrogen bromide is highly corrosive to most metals, and is incompatible with strong oxidizers, caustics, and moisture.

Boron Trichloride. Boron trichloride (BCl_3) is a colorless gas with a pungent odor. BCL_3 has a molecular mass of 117.17 grams per mole (g/mol), and is also a heavy gas. Prolonged exposure to this chemical can impair an individual's ability to escape and potentially cause death. Fumes from BCL_3 can irritate the eyes, affect the central nervous system, and cause shock and coma. Exposure also can cause severe skin burns and can damage organs. Boron trichloride reacts vigorously with water and steam to produce heat, as well as toxic and corrosive fumes. BCl_3 also reacts energetically with various chemicals, such as nitrogen dioxide, tetraoxide, and phosphine.

Carbon Monoxide. Carbon monoxide (CO) is a colorless, odorless, poisonous gas. CO has a molecular weight of28.0 amu, which means it would disperse into the air, rather than accumulating in large masses near the ground, like Cl_2 and HBr. Exposure to large doses of carbon monoxide can be fatal to personnel. In smaller doses, carbon monoxide can also cause headache, nausea, lassitude, dizziness, confusion, and hallucinations. In addition, CO is a flammable gas that can ignite or react when exposed to strong oxidizers, such as bromine trifluoride, chlorine trifluoride and lithium.

The toxic endpoint concentrations for each chemical are shown in parts per million (ppm) in Table 1, below.

Table 1: PAC Values in PPM

Chemical	Current IFSB Value	ERPG-3	ERPG-2	AEGL-3	AEGL-2	PAC-3	PAC-2
Cl_2	20	20	3	20	2	20	2
HBr	30	NA	NA	120	25	120	25
BCl_3	2.7	NA	NA	NA	NA	2.1	2.1
CO	500	500	350	330	83	330	83

In the table, above, "NA" is indicates chemicals for which a toxic endpoint value has not been developed. Toxic endpoint values vary, depending on differences in development processes, differences in definition (i.e., includes vs. does not include hypersensitive individuals), and the hazardous qualities of each chemical. For some chemicals, the endpoint level-2 and -3 are the same (e.g., BCL_3). This data shows a concentration at which a difference in the severity of toxic effects on exposed personnel could not be distinguished. In some cases, a chemical may have the same ppm value for both toxic endpoints at level 3, but have different values at level 2. For example, in Table 1, above, chlorine has a concentration of 20 ppm for ERPG-3 and AEGL-3, but different concentrations at level ERPG-2 and AEGL-2. Variations in concentration values are a result of differences in the definitions of the toxic endpoints, as well as differences in the development processes.

The compared PAC values for each of these chemicals are also shown in Attachment 1, Figures 1-4.

7. IFSB HAZARD CLASSIFICATION CRITERIA

Modeling analyses are used to determine the potential consequences of a toxic gas release to both onsite and offsite receptors. “Low hazard” classification is based on modeling results within 100 m of the release site. Currently, the “moderate hazard” classification is based on modeling results at a distance of 100 m, with a toxic endpoint greater than ERPG-3 with a 15-minute release. “High hazard” classification is based on modeling results at the site boundary, where members of the public could potentially be harmed, with a toxic endpoint greater than ERPG-3 with a 15minute release.

7.1 Areal Locations of Hazardous Atmospheres (ALOHA)

The dispersion model used in this analysis is the Areal Locations of Hazardous Atmospheres (ALOHA) computer program, co-developed by the Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). This program is approved by the Department of Energy, and is generally used by industries for emergency planning and response purposes.

ALOHA is an uncomplicated, user-friendly program used to model chemical hazards (such as toxicity), flammability, heat, and overpressure. ALOHA uses the Gaussian model, and has the ability to model a chemical release from any specific location to estimate the hazardous gas cloud concentrations that would form as a result of that release. For gases that are heavier than air, the ALOHA model assumes that the gas will fall to the ground before reaching the distance of concern, and, thus, does not model an elevated release. ALOHA minimizes errors by checking the input parameters, and alerts the user if a mistake is made. The program also runs quickly, because it is designed to operate in high-pressure situations. However, when modeling at less than 100 m, ALOHA is not considered to be accurate. For this reason, IFSB analysts limit the program use to the acquisition of comparative values when determining a facility’s initial hazard classification.

In ALOHA, a user can choose AEGLs, ERPGs or PACs (TEELs) as the toxic Levels of Concern (LOCs) when modeling a toxic chemical release— if the toxic endpoint has been defined for that chemical. ALOHA allows up to three specified toxic LOCs. For example, an analyst can choose the AEGL-1, AEGL-2, and AEGL-3 values to generate a "threat zone" estimate, where yellow, orange, and red indicate the zones in which LOC values are predicted to be exceeded at some point during the chemical release.

A particular chemical may have values in any, or all, of these exposure guidelines. If final or interim AEGLs are available for the chemical being modeled, ALOHA will provide the AEGL values, with a 60-minute exposure duration as the default toxic LOCs. If AEGLs are not available, ALOHA will default to the ERPG values, and then to the PAC values, which are created by the TEEL developers (i.e., DOE and SCAPA). The PAC dataset combines all three public exposure guidelines and implements a hierarchy-based system for the user. If ALOHA defaults to the PAC values, it means that there are no AEGL or ERPG values in the ALOHA chemical library for that substance. In this case, the PAC values will be the TEEL values.

7.2 IFSB/ALOHA Modeling Parameters

IFSB provides general parameters for use in various ALOHA studies.

The IFSB modeling protocol assumes a release over a 15-minute (min) time period, even though the ERPG-3 endpoint is based on a 60-min impact period. This modification was made because a catastrophic chemical release would take place in 15 minutes or less, rather than over a 1-hour period of time. The 15-minute release duration is used as an ALOHA modeling parameter and is based on the Temporary Emergency Exposure Limits (TEEL) values. Because these values are based on the 15-minute release duration, a similar release duration methodology of 15 minutes had to be applied to the AEGL and ERPG values for them to remain comparable. When this methodology is applied to the AEGL and ERPG values, it is referred to as having a "safety factor of 4" (60-min/4 = 15 min). The 15-minute release duration (safety factor of 4) is commonly accepted throughout the DOE complex by members of EFCOG (Energy Facility Contractors Group), and although this practice is widely accepted, its origin and derivation are not explicitly contained within any identifiable guidance documentation. In this analysis, PAC values are compared to the AEGL and ERPG values for both a 15-minute and a 60-minute release period.

IFSB modeling parameters reflect worst-case scenario meteorology and include an override input value "F" (95%) stability class. This meteorology adds a layer of conservatism both when analyzing toxics hazards and when classifying facilities.

Table 2, below, presents the general parameters used in ALOHA for various studies, as well as the IFSB modeling protocol specific to this analysis.

Table 2: IFSB/ALOHA Modeling Parameters

Variable	Model Input
Location	Kirtland AFB, NM
Wind Speed	1.5 meters/second (m/s)
Wind Direction	East (E)
Wind Tower Height	10 meters (m)
Ground Roughness	Open Country
Cloud Cover	Clear
Air Temperature	20° C
Stability Class – 95%	F (Override)
Inversion Height	300 m
Humidity	25%
Source Height	0 m
Release Quantity	x pounds (lbs)
Release Period	15 min or 60 min
Release Rate	x/15 lbs/min

7.2.1 Wind Speed

IFSB protocol establishes 1.5 meters per second (m/s) as the wind speed input parameter. The wind speed affects how fast a gas cloud would travel downwind, and how much the cloud would move (approximately) in crosswind and vertical directions. Between 1 m/s and 2 m/s, the wind speed is internationally described as "Light Air" (ALOHA Manual 2007), meaning that 1) there would be little-to-no mixing, and 2) gas would accumulate in larger, more hazardous concentrations. Based on model runs, higher wind speeds result in closer distances to the LOC. ALOHA sets 1 m/s as its minimum wind speed value, at which the gas cloud results in the farthest distance.

7.2.2 Wind Direction

The wind direction parameter determines which way a gas cloud will drift following a release. IFSB analysts can use different directions for specific studies, or can use the value "0" to evaluate a release in all directions. Based on modeling runs, the wind direction does not affect the distance to the LOC.

7.2.3 Wind Tower Height

uses a pattern called a "wind profile" to observe changes in the wind speed depending on elevation. The profile, expressed in Figure 1, below, shows that friction slows the wind closer to the ground. As the elevation rises, the wind speed increases until it reaches a maximum, at which point it is no longer affected by friction. The height above the ground where surface friction has a negligible effect on wind speed is called the "gradient height." The wind speed above this height, assumed to be a constant, is called the "gradient wind speed."

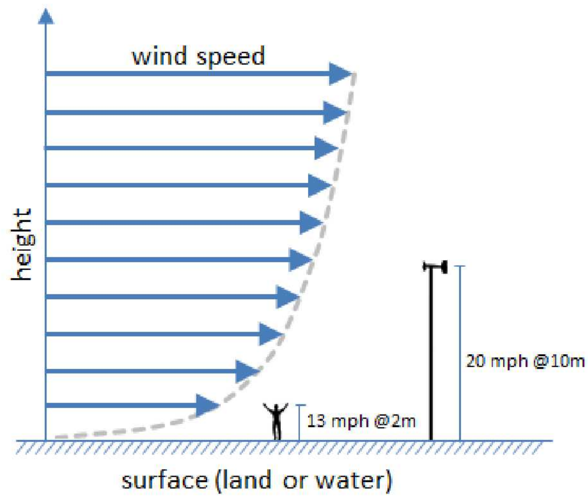

Figure 1: Wind Profile

As a note, the National Weather Service usually reports the use of a measurement height of 10 meters when determining wind speed. IFSB protocol is to use 10 meters when modeling a catastrophic release.

7.2.4 Ground Roughness

A user has four selection options in ALOHA relating to ground roughness. These include "Open Country," "Urban or Forest," "Open Water," and a "User Input" option. For each option there are varying degrees of atmospheric turbulence that influence how quickly a pollutant cloud will dilute due to air mixing. Surface roughness is determined from the number and the size of the elements present in the evaluated area, and results in greater degrees of turbulence. IFSB protocol assumes an Open Country ground roughness parameter having minimal roughness elements in the area and a low degree of turbulence. During modeling runs, the Open Country parameter results in farther distances to the LOC; whereas, the Urban or Forest option causes a gas cloud to dilute at a distance below the selected LOC.

7.2.5 Cloud Cover

When modeling a puddle release in ALOHA, it is important to enter a particular value for "cloud cover" to estimate the influence of solar radiation on the puddle evaporation rate . However, in the event of a direct gas release, results from modeling runs show that cloud cover does not affect the distance to the LOC for the screening chemicals. IFSB assumes a "Clear" sky parameter, based on the average meteorological data for the area.

7.2.6 Air Temperature

Similar to cloud cover, the air temperature parameter is significant when modeling a liquid puddle release, because it relates to the evaporation rate from the puddle surface. Based on modeling runs for a direct release, chemicals are affected differently by temperature, soit is important to have an accurate temperature value. However, the results from the screening chemicals are not significantly affected by temperature. IFSB uses 20^{o} Celsius, because it corresponds to the average temperature of the evaluated area.

7.2.7 Stability Class

Meteorologists have defined six stability classes, representing varying degrees of turbulence in the atmosphere depending on the amount of incoming solar radiation, wind speed, and other factors. The classes range from A (unstable) to F (stable). When strong, incoming solar radiation heats air near the surface, causing it to rise and flow in circular movements, the atmosphere has high turbulence and is considered unstable. When solar radiation is weak or absent, air near the ground has a reduced tendency to rise, and the atmosphere has low turbulence. This condition, along with low wind speeds, would present a stable atmosphere.

Stability class has a significant influence on the threat zone size and distance to the LOC for dispersion scenarios. Modeling results show that, in unstable atmospheres (stability class "A"), a gas cloud would disperse quickly as it is diluted by turbulence and mixed with air, so the distance to the LOC would be shorter. Oppositely, using stability class F, which represents a 95% stable atmosphere, results in the farthest distance to the LOC for any given chemical. This data shows that on hot, windy days, a gas cloud would disperse quickly into the air. On cool, calm nights, however, a pollutant cloud would reach its farthest potential distance. IFSB uses the "F" stability class to model a release based on a worst-case meteorological condition.

Figure 2 (below) shows the differences in atmospheric conditions (ALOHA Manual, 2007).

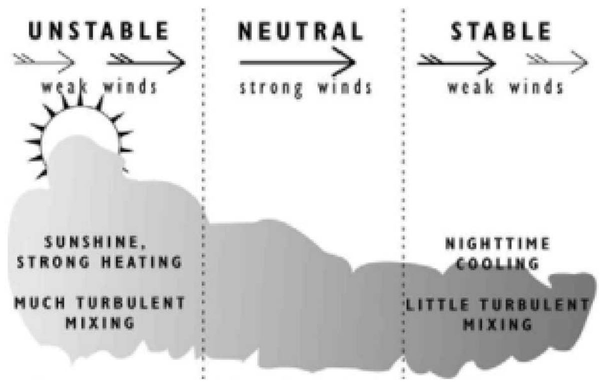

Figure 2: Atmospheric Conditions

7.2.8 Inversion Height

An "inversion" is an atmospheric condition in which an unstable layer of air near the ground lies below a very stable layer of air above. Inversions are more often present in large cities, in valleys, and at night— all of which are factors present in this analysis. The height at which the abrupt change in atmospheric conditions occurs is known as the "inversion height," and it can be different or absent, depending on the location and other factors. Inversion height is important to take into account when modeling a chemical release, because an inversion can trap gases and cause concentration levels to reach higher levels near the ground. A low-level inversion may significantly increase ground-level concentrations of a neutrally buoyant gas, because it reflects molecules of such gases back toward the ground. A heavy gas cloud, in contrast, remains close to the ground as it disperses and is not normally affected by any inversion height.

This data is represented in modeling results that show carbon monoxide (CO) was affected by varying inversion heights while chlorine, a heavy gas, was not. For example, at a 15-m inversion height, CO resulted in a larger distance of 800 m, although, with a larger inversion height, the distance to the LOC was shorter. IFSB analysts and meteorological specialists decided on an inversion height of 300 m, as it relates to atmospheric conditions in the evaluated area.

7.2.9 Humidity

Relative humidity is the amount of water vapor that the air contains compared to the maximum amount that the air could hold at ambient temperature and pressure. ALOHA uses humidity to estimate the rate of evaporation, which is significant when modeling puddle releases. Based on the modeling results for a direct release, in contrast, the distance to the LOC was the same, despite changes in the humidity parameter. IFSB assumes a 25% relative humidity based on meteorological data for the evaluated area.

7.2.10 Source Height

IFSB models dispersion scenarios using a source height of 0 m, that is, as if the release is happening at ground level. At ground level, the gas will disperse farthest, because it will move out in different directions, and up instead of down. Especially for heavy gases, it is important to model using a source height of 0 m, because ALOHA is more accurate under these parameters.

8. RESULTS

Tables 3-6 (below) show the quantity results in pounds for back calculations at 100 meters for each of the screening chemicals. The toxic endpoints and corresponding quantity values shown in **bold** express a potential impact to the hazard classification, because they are below the current threshold level. These threshold levels can be found in Question 5K of the Primary Hazard

Screening (PHS), and are the inventory standard for classifying SNL facilities based on chemical releases.

Table 3: Chlorine

15-minute Release Period					
ERPG-3	**ERPG-2**	**AEGL-3**	**AEGL-2**	**PAC-3**	**PAC-2**
3.75 lbs	**0.447 lbs**	**3.75 lbs**	**0.293 lbs**	**3.75 lbs**	**0.293 lbs**

The current threshold level for chlorine is 6.29 lbs. For a 15-minute release, all toxic endpoints resulted in a quantity below the current threshold level. This data suggests that using any of the screened toxic endpoints at a 15-minute release could potentially result in a jump in hazard classification from a Low level to a Moderate level for SNL facilities storing chlorine. Refined analysis would determine the exact values. (Attachment 1: Figure 5)

60-minute Release Period					
ERPG-3	**ERPG-2**	AEGL-3	**AEGL-2**	PAC-3	**PAC-2**
15 lbs	**1.79 lbs**	15 lbs	**1.17 lbs**	15 lbs	**1.17 lbs**

For a 60 minute release, toxic endpoints at level -2 resulted in a quantity below the current threshold level. For ERPG-3, AEGL-3 and PAC-3 at 60 minutes, the quantity exceeded the current threshold level. The modeling runs show that the updated protocol, using PAC-3 as the screening criterion would increase the threshold level for chlorine from the current 6.29 lbs to 15 lbs. A significant increase in threshold level could potentially drop facilities from a Moderate to a Low hazard classification depending on chemical inventory. To maintain a similar number of low and moderate facilities (based on current "right-size of program), a jump from 6.29 lbs to 15 lbs in quantity thresholds should be further analyzed to understand all impacts to the hazard classification. (Attachment 1: Figure 5)

Table 4: Hydrogen Bromide

15-minute Release Period					
ERPG-3	ERPG-2	AEGL-3	**AEGL-2**	PAC-3	**PAC-2**
NA	NA	49.5 lbs	**6.3 lbs**	49.5 lbs	**6.3 lbs**

No current ERPG values are derived for hydrogen bromide. The current threshold level for hydrogen bromide is 11.72 lbs. For a 15-minute release, modeling runs for AEGL-2 and PAC-2 resulted in a quantity below the current threshold level. This data suggests that using AEGL-2 and PAC-2 as updated protocol at a 15-minute release could potentially result in a jump in hazard classification from Low to Moderate for SNL facilities storing hydrogen bromide. Refined analysis would determine exact values. AEGL-3 and PAC-3, in contrast, resulted in quantities above current threshold level, showing no/limited impact to the hazard classification. (Figure 6)

60-minute Release Period					
ERPG-3	ERPG-2	AEGL-3	AEGL-2	PAC-3	PAC-2
NA	NA	198 lbs	25.2 lbs	198 lbs	25.2 lbs

No current ERPG values are derived for hydrogen bromide. For a 60-minute release, quantities for toxic endpoints AEGL-2, AEGL-3, PAC-2 and PAC-3 exceeded the current threshold level. The modeling runs show that using the updated PAC-2 protocol using as screening criteria would increase the threshold level for hydrogen bromide from the current 11.72 lbs to 25.2 lbs. The modeling runs show that the updated protocol using PAC-3 as screening criteria would increase the threshold level for hydrogen bromide from the current 11.72 lbs to 198 lbs. This difference should be further analyzed, as a large jump in quantity thresholds has the potential to impact the hazard classification for facilities storing hydrogen bromide. (Attachment 1: Figure 6)

Table 5: Boron Trichloride

15-minute Release Period					
ERPG-3	ERPG-2	AEGL-3	AEGL-2	**PAC-3**	**PAC-2**
NA	NA	NA	NA	**0.53 lbs**	**0.53 lbs**

No current ERPG or AEGL values are derived for boron trichloride. The current threshold level for boron trichloride is 1.15 lbs. For a 15-minute release, modeling runs for PAC-2 and PAC-3 resulted in a quantity below the current threshold level. This data suggests that using PAC-2 and PAC-3 as updated protocols at a 15-minute release could potentially result in a jump in hazard classification from a Low level to a Moderate level for SNL facilities storing boron trichloride. A refined analysis would determine exact values. (Attachment 1: Figure 7)

60-minute Release Period					
ERPG-3	ERPG-2	AEGL-3	AEGL-2	PAC-3	PAC-2
NA	NA	NA	NA	2.1 lbs	2.1 lbs

No current ERPG or AEGL values are derived for boron trichloride. For a 60-minute release, quantities for toxic endpoints PAC-2 and PAC-3 exceeded the current threshold level. The modeling runs show that the updated protocol, using PAC-2 or PAC-3 as screening criteria, would increase the threshold level for hydrogen bromide from the current 1.15 lbs to 2.1 lbs. (Attachment 1: Figure 7).

Table 6: Carbon Monoxide

15-minute Release Period					
ERPG-3	**ERPG-2**	**AEGL-3**	**AEGL-2**	**PAC-3**	**PAC-2**
21 lbs	**14.6 lbs**	**13.65 lbs**	**3.45 lbs**	**13.65 lbs**	**3.45 lbs**

The current threshold level for carbon monoxide is 96.47 lbs. For a 15-minute release, all toxic endpoints resulted in a quantity below the current threshold level. This data suggests that using any of the screened toxic endpoints as updated protocols at a 15-minute release could potentially result in a jump in hazard classification from a Low level to a Moderate level for SNL facilities storing carbon monoxide. Refined analysis would determine the exact values. (Shown in Attachment 1: Figure 8)

60-minute Release Period					
ERPG-3	**ERPG-2**	**AEGL-3**	**AEGL-2**	**PAC-3**	**PAC-2**
84 lbs	**58.2 lbs**	**54.6 lbs**	**13.8 lbs**	**54.6 lbs**	**13.8 lbs**

For a 60-minute release, all toxic endpoints resulted in a quantity below the current threshold level. This data suggests that using any of the screened toxic endpoints as updated protocols at a 60-minute release could potentially result in a jump in hazard classification from a Low level to a Moderate level for SNL facilities storing carbon monoxide. Refined analysis would determine exact values. (Shown in Attachment 1: Figure 8)

In this study, PAC values were evaluated to determine the impact on the IFSB hazard classification as a result of different toxic endpoint levels and release times. Results for PAC-2 at 15 minutes yielded a significant change to the current (historic) primary hazard screening (PHS) question 5k threshold values for toxics. PAC-2 at 60 minutes and PAC-3 at 15 minutes result in quantities that are not similar to those derived using the current methodology at 100 m. The chemical quantities at these endpoints show results below the current threshold level. It is concluded that using PAC-2 and PAC-3 at 15-minute releases, and PAC-2 at a 60-minute release, could potentially cause the hazard classifications of facilities at the SNL site to increase from low to moderate. In contrast, the modeling results for three of the four chemicals show that PAC-3 at 60 minutes could be used as new protocol without significant impacts to current facility hazard classifications. Of the four screening chemicals, only the threshold value for carbon monoxide dropped below the current ERPG-3-based threshold value. Based on this new toxic endpoint, facilities using carbon monoxide could potentially be impacted; however, a refined analysis would determine a final quantity that could be compared to the current threshold values. Based on modeling runs, the toxic endpoint having results most similar to those derived with the current methodology is PAC-3 at a 60-minute release period.

9. CONCLUSION

IFSB currently uses ERPG values derived from historic (i.e., 2006) values as the standard for determining hazard classification (as stated in PLA 05-03 and the IFSB Guidance Document). These historic values are based on analysis and calculations using the ERPG-3 and TEEl-3 values of record at the time of the analysis. Many ERPG-3 values have now been updated and published by SCAPA based on current and more refined data, although the historic values are still used as protocol for IFSB hazard classification. The current IFSB methodology uses a safety factor of 4 (15 minute release), and is based on modeling using worst-case scenario parameters. These parameters give an added layer of conservatism to the IFSB modeling protocol. It is important for IFSB to be both conservative and realistic when determining hazard classification to 1) ensure that workers, collocated workers, and the public are safe, and 2) that facilities are efficient and productive in executing their processes and projects.

In comparison to the derived IFSB ERPG-3 values, PAC values are more readily available for use in emergency planning, and include values for all chemicals (SCAPA). PAC values (corresponding to AEGLs) are derived from primary toxicological information, and are based on current data from human and animal studies. These values are currently assumed to be the most accurate public exposure guidelines available. With new screening criteria based on more-refined data, personnel will have more control to implement safety factors as needed. An updated protocol establishing PAC-3 at 60 as the classifying methodology would render more realistic modeling results, because the toxic endpoint is more precise at an hour-long release period. The 15-minute release period currently in use adds a layer of conservatism to modeling analyses; however, a safety factor of 4 is no longer needed in modeling analysis, based on more accurate results and other layers of conservatism that include sensitive individuals and worst-case meteorological data.

PAC values corresponding to AEGLs and TEELs have a level of conservatism that includes toxic effects on hypersensitive individuals, such as children, the elderly, and those with asthma or weaker immune systems. These individuals are generally not considered in emergency planning, but should be taken into account when modeling to ensure that the workers, co-located workers, and the public are appropriately protected. This safety factor would be automatically implemented in conjunction with the updated protocol. In addition, IFSB modeling parameters provide a thick layer of conservatism, because the variables are based on a worst-case scenario, including an override input parameter (F-stability class) that would, realistically, only take place at night. In addition to the levels of conservatism built into the IFSB modeling protocol, there are preventive and mitigative controls in place at each facility to protect personnel following a release, although those controls cannot be established as conservative. Preventive controls at facilities, which attempt to stop a release scenario from taking place, consist of process regulations, such as restricting the unloading of chemical cylinders during evening hours. The mitigative controls in place consist of alarms and evacuation plans that aid personnel to reach a place of safety in the event of a release.

Based on the current IFSB model, it is assumed that there are an appropriate number of moderate versus low hazard facilities at Sandia. The current program is considered to be "right- sized". Adopting new toxic threshold values that establish the 858 Complex (Microsystems Engineering and Sciences Applications, or MESA) as a low-hazard facility would raise concern due to the chemical inventory and the distance of the facility from the site boundary; this would likely mean that the threshold values used were set too high. In contrast, adopting new toxic threshold values that showed building 823, which predominantly consists of office rooms with a few labs, as a moderate facility could be considered excessive and would likely mean the threshold values used were set too low. In the event that threshold values were set too low, there would likely be many new "moderate" facilities. As numerous moderate facilities are identified, extensive refined analyses would have to be conducted on a regular basis. A surge in the number of analyses could require both an increase in budget and additional team members for IFSB.

Based on modeling runs, it is concluded that PAC-3 at 60 minutes is most similar to the current methodology and, if used as an updated IFSB protocol, is likely to result in a similar number of moderate hazard facilities (based on chemical classification alone). Based on research, it is concluded that PAC-3 at 60 minutes is acceptable to use as a classification criterion based on

1) the availability and accuracy of PAC values,
2) the layer of conservatism that includes hypersensitive individuals, and
3) other layers of conservatism, including worst-case modeling parameters.

10. RECOMMENDATIONS

Based on the conclusions presented above, it is recommended that PAC-3 at 60 minutes be accepted as the new IFSB methodology for classifying facilities based on chemical release scenarios.

Further analysis through model runs using a larger sampling of chemicals is needed to fully understand the potential impacts on the hazard classification for the SNL/NM site. An augmented study is recommended, for a safety analyst to reference this report, as well as previous analyses, and conduct model runs for each chemical on the Standard Toxic Gas List (located in PHS Q5k help text). An analyst could then run CIS toxics pulls for the entire SNL/NM site and compare the new threshold values to the old historic values and determine how many, and which particular, buildings have the potential to jump from a Low to a Moderate hazard classification. If further analysis reflects modeling results similar to those included in this report, and if modeling conclusions show that PAC-3 at 60 minutes as the toxic endpoint would have limited impacts on hazard classification and associated changes (with results similar to the current "right-size" program), the IFSB team will determine the next steps required to update the protocol.

APPENDIX A: TOXIC END POINT VALUES

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Figure A-1: Chlorine – Cl2

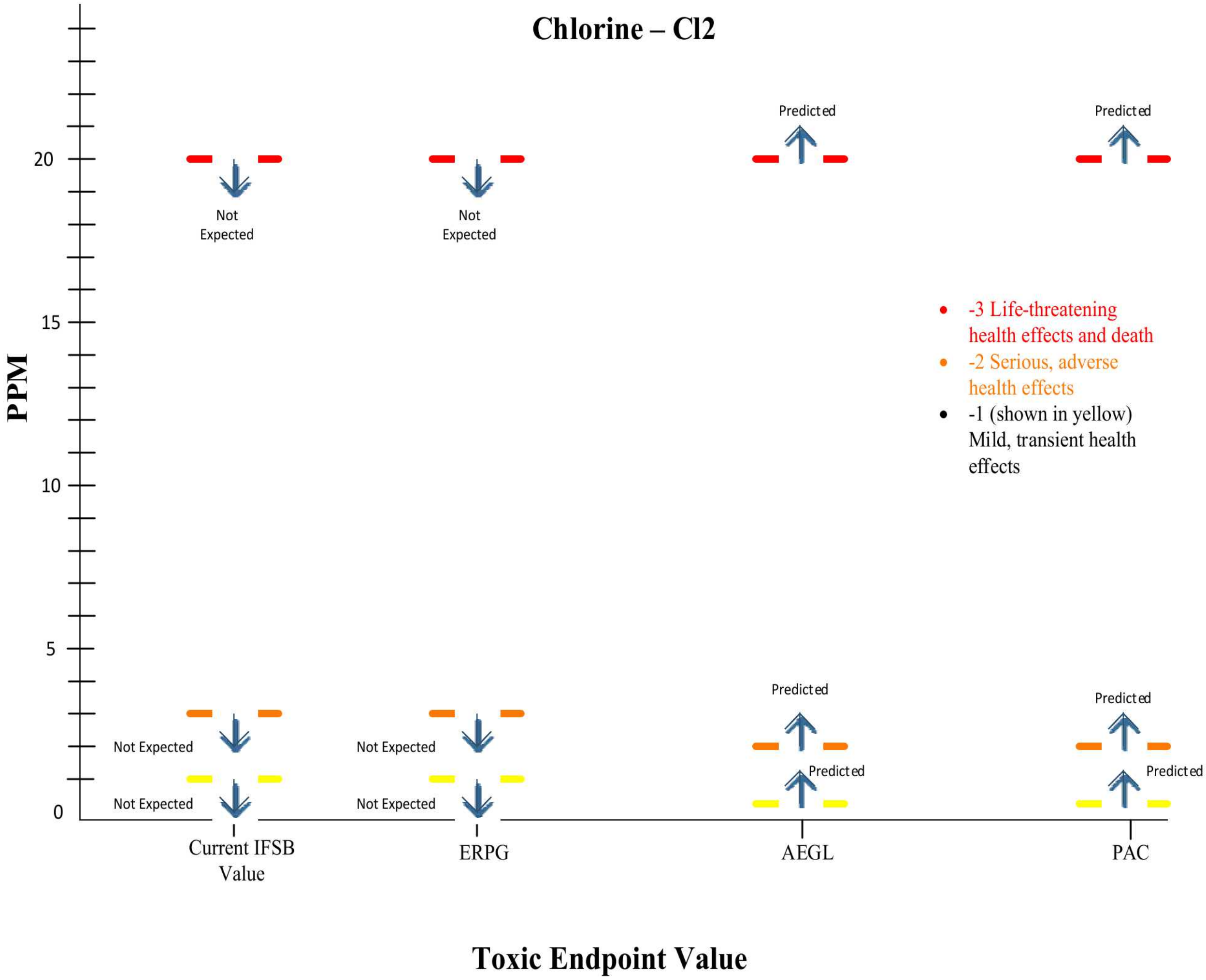


Figure A-2: Hydrogen Bromide – HBr

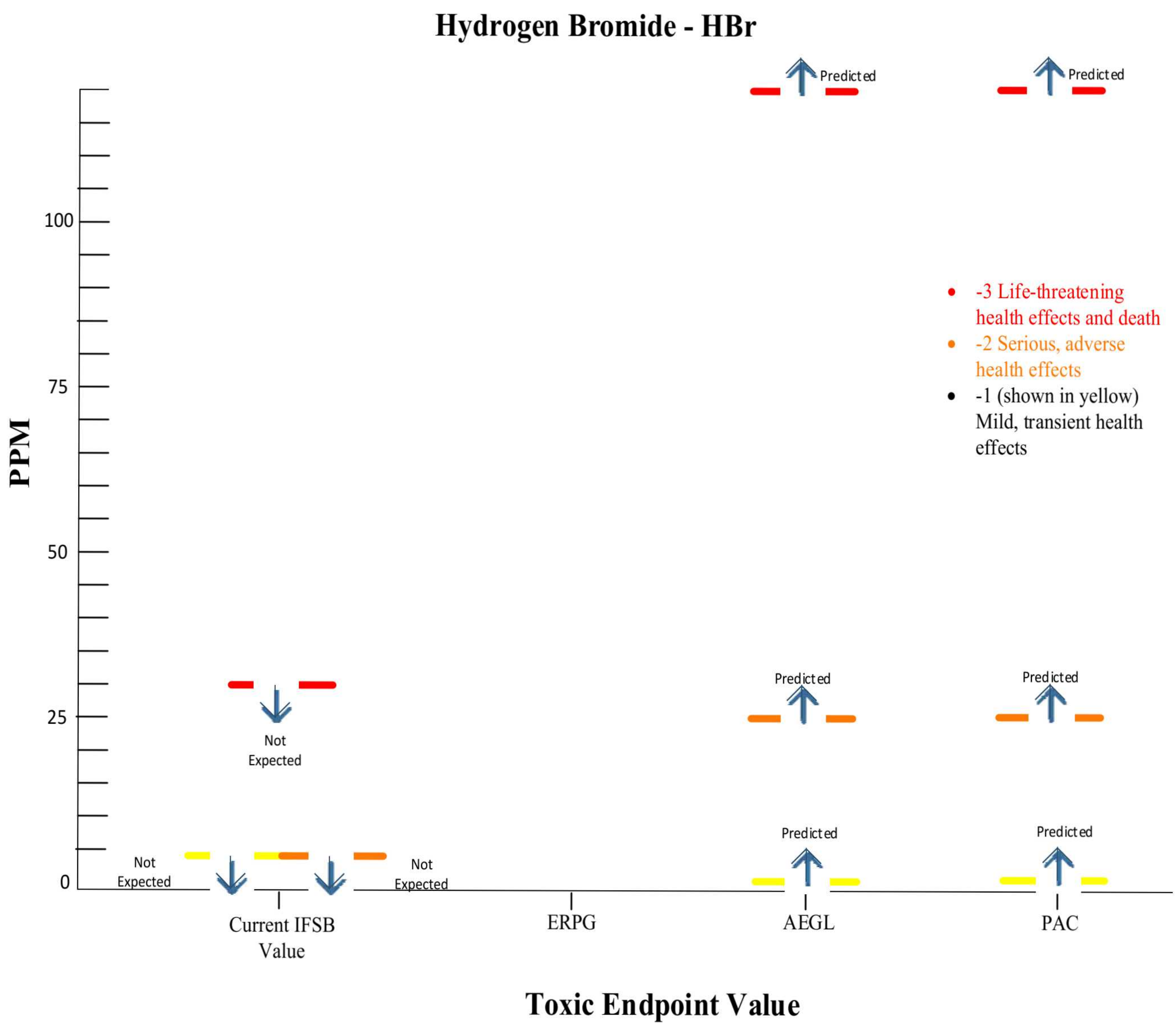


Figure A-3: Boron Trichloride – BCl3

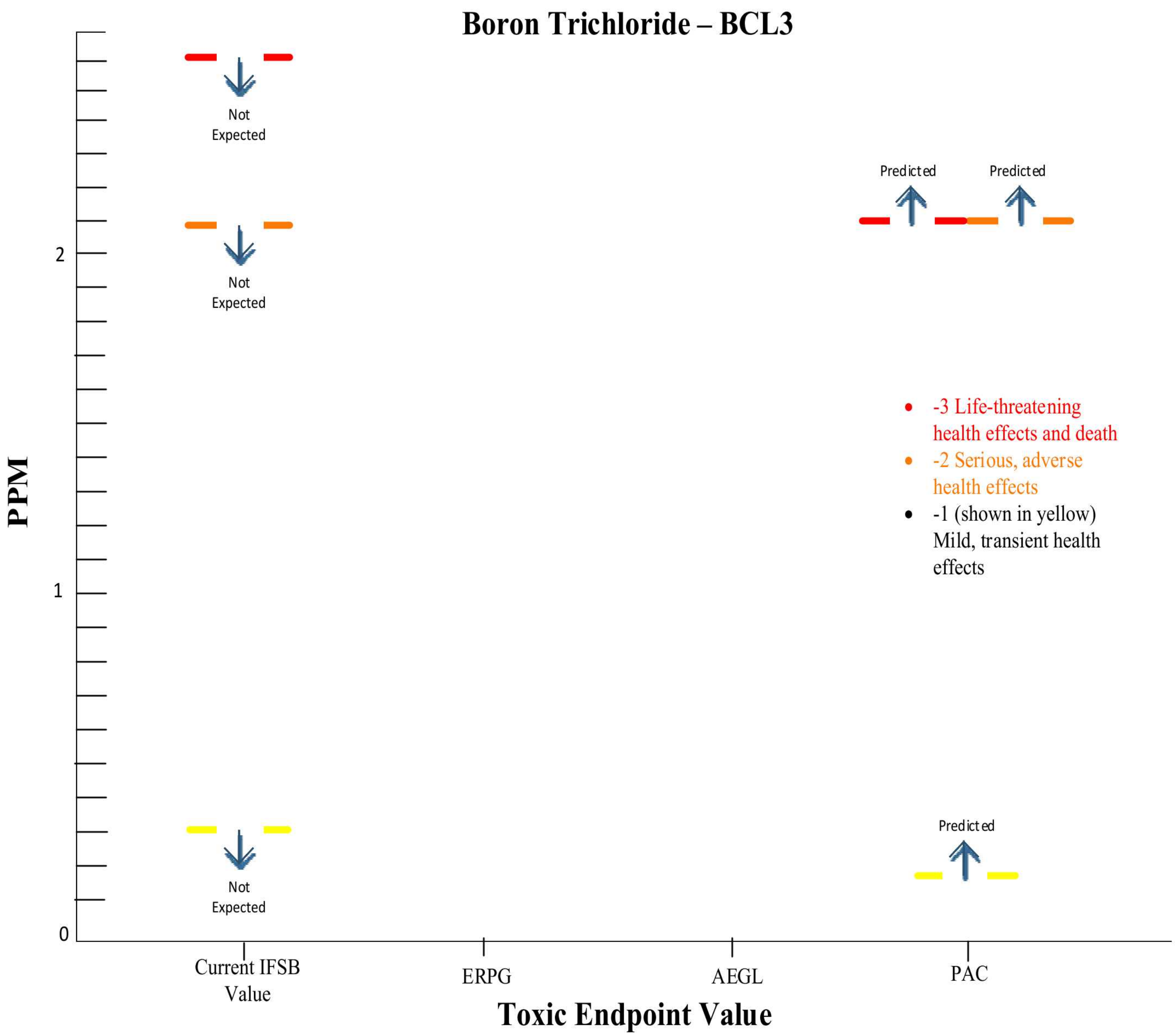


Figure A-4: Carbon Monoxide (CO2) - 100 m

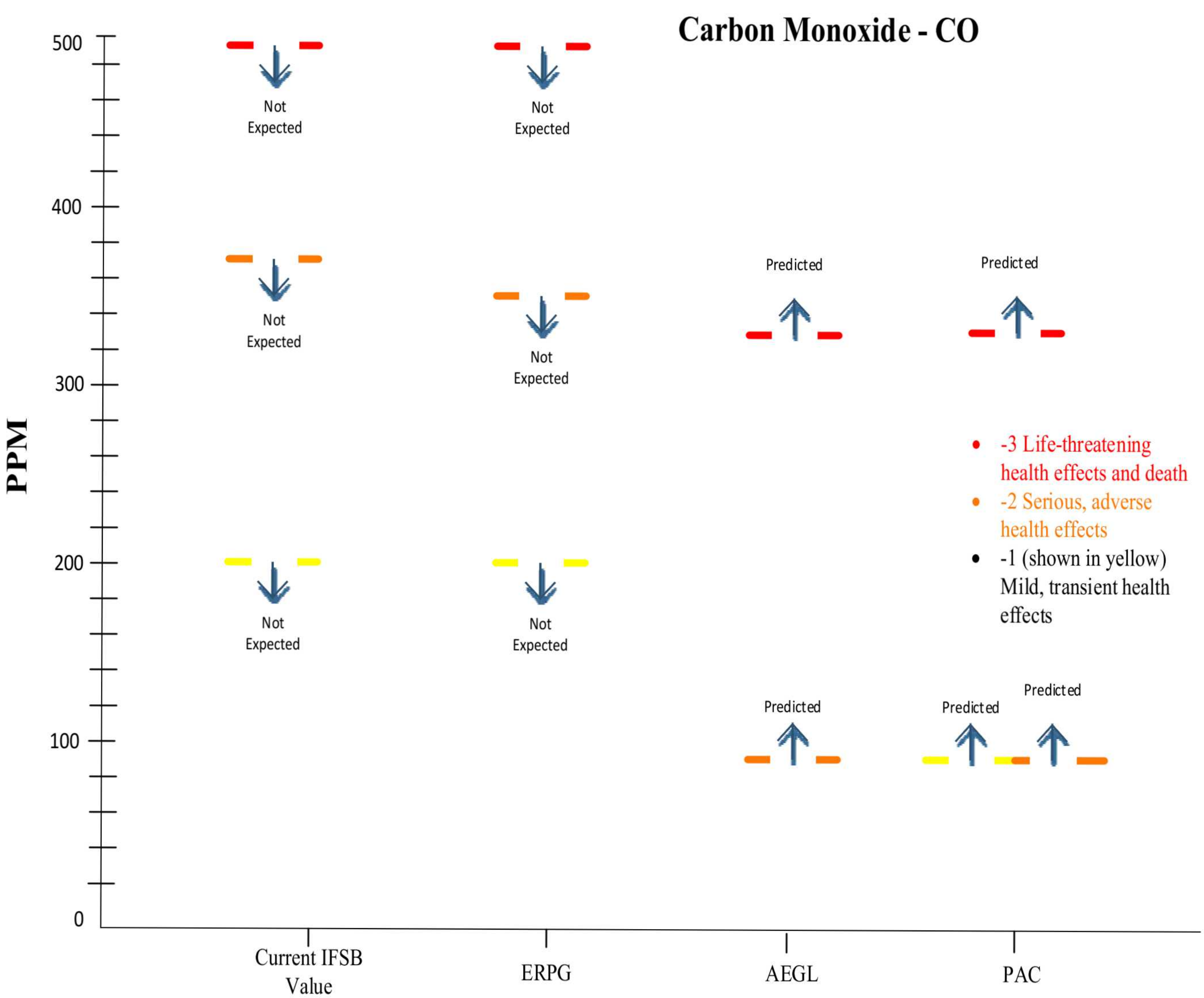


Figure A-5: Chlorine (Cl2) – 100 m

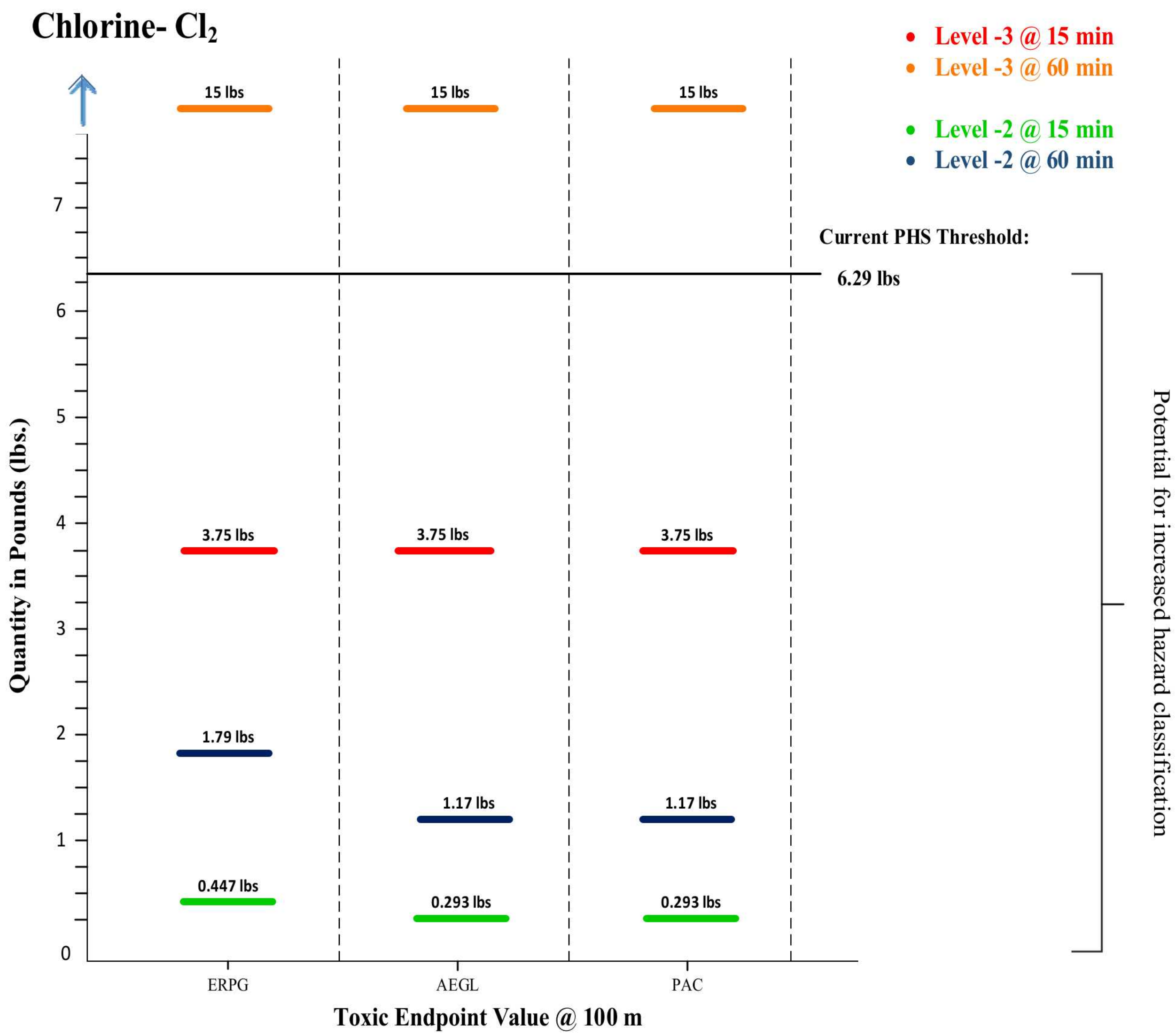


Figure A-6: Hydrogen Bromide (HBr) – 100 m

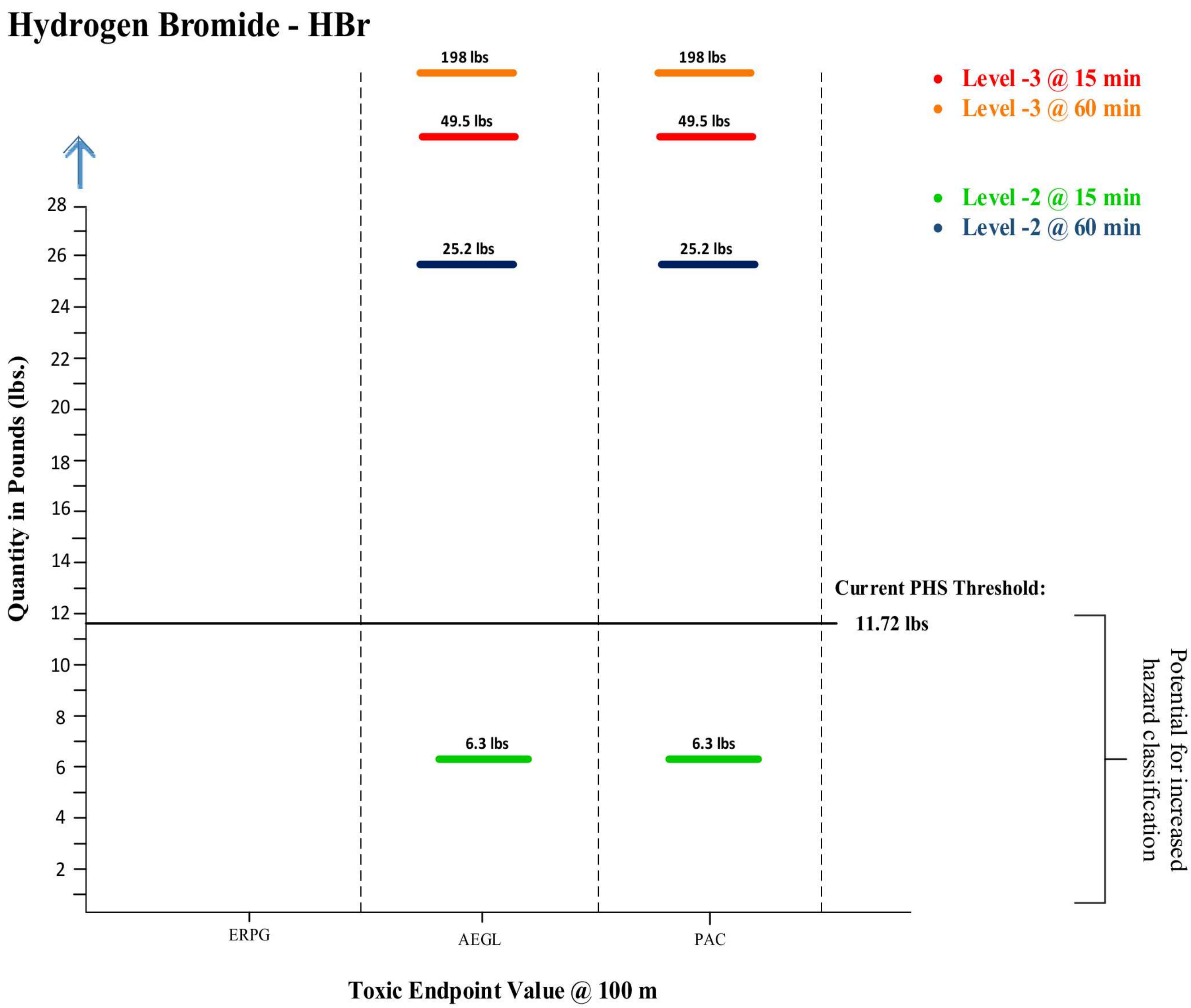


Figure A-7: Boron Trichloride (BCL3) – 100 m

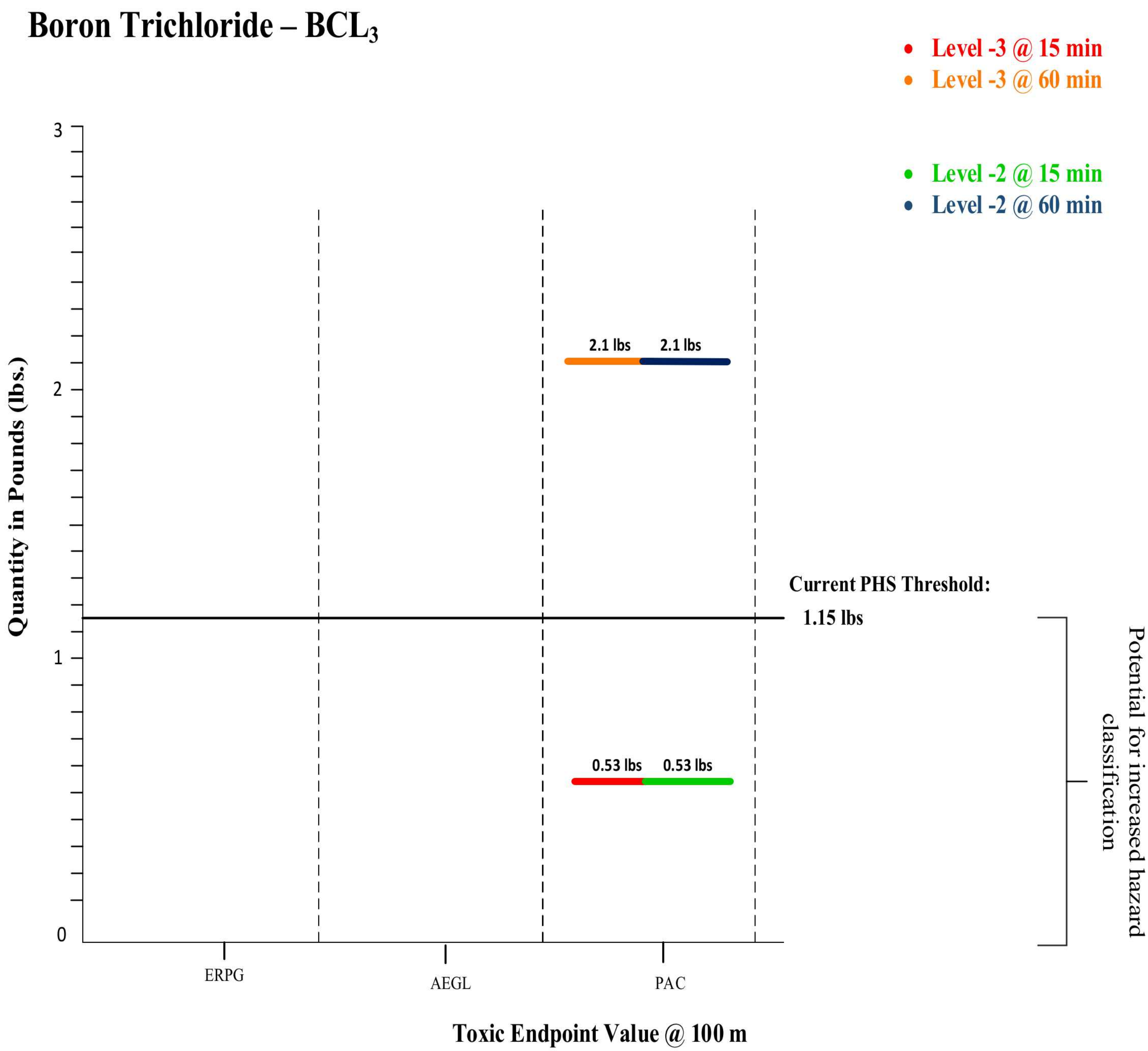
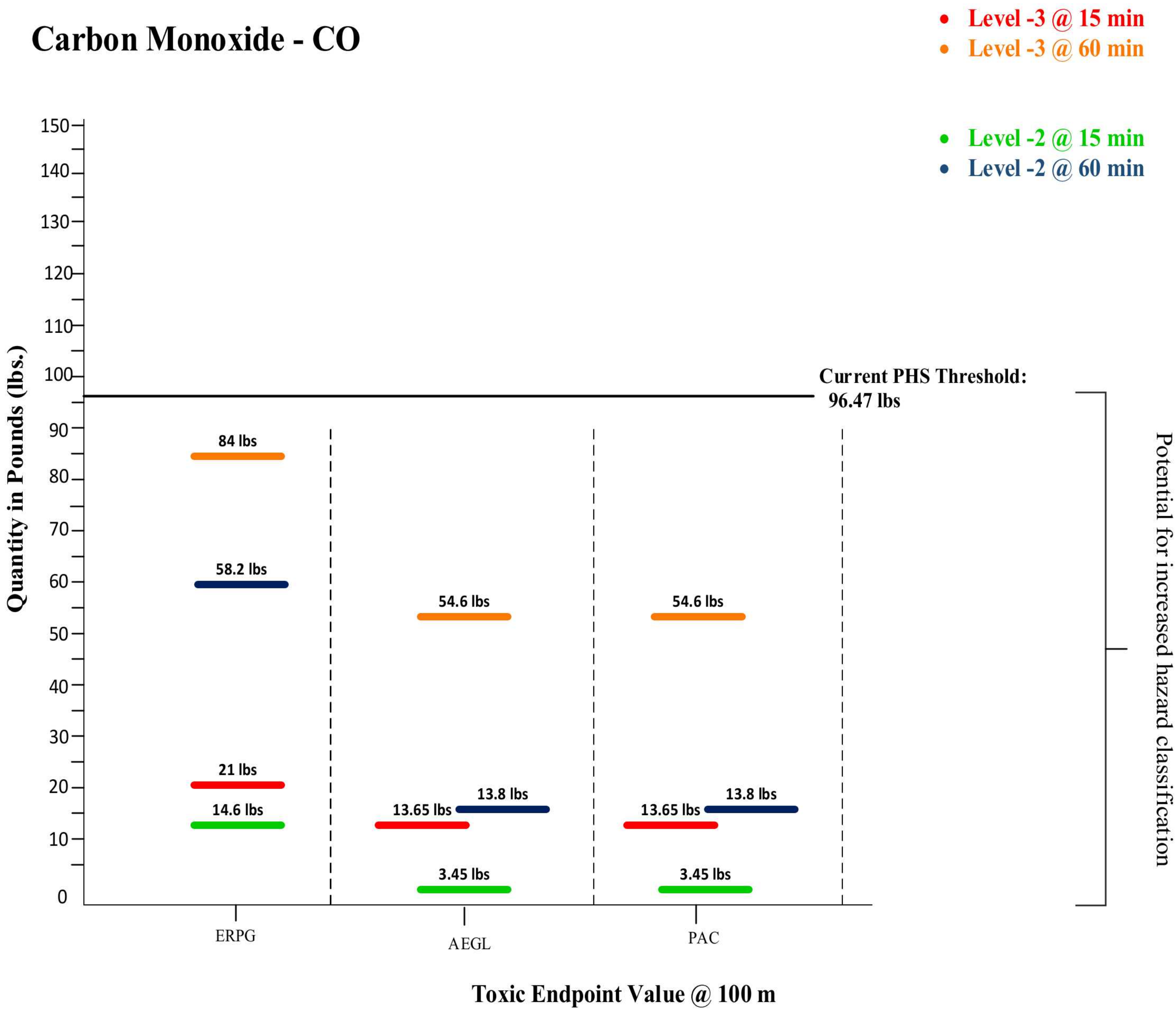


Figure A-8: Carbon Monoxide (CO) – 100 m



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