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Application of Statistical Cross-Extrapolation Techniques to Derive Surrogate Acute Exposure Guideline Levels (AEGLs)

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Abstract

Application of Statistical Cross-Extrapolation Techniques to Derive Surrogate Acute Exposure Guideline Levels (AEGLs)

By MyDzung T. Chu

AEGLs are comprehensively peer-reviewed health guidance values (HGVs) for assessing the risk of acute once-in-a-lifetime or rare exposures to hazardous inhalation chemicals. For each inhalation compound, up to fifteen AEGL values may be developed that address three health effects severity thresholds (AEGL-1: discomfort/reversible, AEGL-2: disabling/irreversible, AEGL-3: life threatening) at five exposure durations (1/6, 1/2, 1, 4, and 8 hours). Currently, only 74 compounds have Finalized AEGLs, while 187 are Interim and 12 are Proposed. Among these, 42% have unassigned AEGLs due to insufficient data or biological implausibility of estimates. Also as of November 2011, the AEGL Program no longer reviews new compounds. Therefore, a need for a rapid and cost-effective substitute for AEGL development is imminent. The aim of the present work was to develop an efficient method for the derivation of provisional AEGLs for inhalable hazardous compounds with unassigned AEGLs. Such method is plausible due to uniformity of procedures by which the AEGLs have been developed, and due to similarities in the physical-chemical characteristics of inhalable compounds.

Qualitative and quantitative data for AEGLs were derived from the US Environmental Protection Agency's published technical support documents. Pearson correlation and Deming linear regression (DLR) analyses of the AEGL database were employed to develop a total of 105 unique univariate cross-extrapolation models for duration-and-threshold-specific AEGLs. 95% confidence and prediction intervals (CIs and PIs) of each model were constructed using bootstrap resampling. The most predictive DLR models were applied to compounds with unassigned AEGLs. Obtained estimates were externally validated using other available health guidance data, including occupational exposure limits (OELs) Model performance was also internally validated by comparing estimated and actual AEGLs for compounds with the full set of data.

All Pearson correlation coefficients (*r*) were greater than 0.88. Higher coefficients generally corresponded to cross-extrapolation models with narrower 95% PIs. The narrowest PIs, i.e. the most confident cross-extrapolation, were observed for pairs of AEGLs that were most similar in exposure duration and severity of health effects. Conversely, the widest PIs were obtained for functionally most distant AEGL pairs; however, even the worst estimates were within two orders of magnitude of the actual values. Comparison of estimated AEGLs to occupational HGVs suggested that numerically STELs and TWAs were more correlated with AEGL-1 and -2s at 4 h and 8 h. External validation of cross-extrapolated numbers against these occupational HGVs for a test set of 14 chemicals showed statistical identity at the 95% level for 8 of the 14 compounds.

Our findings suggest that the DLR models are statistically valid and predictive of unassigned AEGL values for compounds in the database. Model performance is dependent on the severity threshold and exposure duration of the cross-extrapolated quantities. External validation using occupational HGVs shows that our cross-extrapolation estimates are sound. Yet, the uncovered relationships are not fully vetted; in particular, our understanding of cross-threshold extrapolation is still emerging, since the involved health endpoints and exposure durations vary on case-by-case basis. Nevertheless, with the lack of short-term exposure HGVs and funding cutbacks in the AEGL Program, the need for surrogate risk assessment methods is ever-growing. In the future, structure-activity, time-scaling, and the biological plausibility of AEGL predictions will be investigated, which may explain the observed high correlations and log-linearity across exposure durations and severity thresholds established in the present study.

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I. INTRODUCTION

Acute Exposure Guideline Levels (AEGLs) are comprehensively peer-reviewed protective action criteria for assessing the risk of acute once-in-a-lifetime or rare exposures to hazardous inhalation chemicals. Developed by an international panel of public and private stakeholders, AEGLs are often employed for assessing health risks and ensuring the safety of first responders, servicemen, and the public during an emergency response, such as to a chemical spill. For each inhalation compound, up to fifteen AEGL values may be developed that address three health severity thresholds (AEGL-1: discomfort/reversible, AEGL-2: disabling/irreversible, AEGL-3: life threatening) at five exposure durations (10 min, 30 min, 1 h, 4 h, and 8 h). Development of AEGL values is ongoing as new chemicals are nominated for review. Most of the data for AEGLs, especially for AEGLs-2 and AEGLs-3, are derived from animal toxicological studies and extrapolated to health protective levels for humans by applying dose/time extrapolation and additional uncertainty factors. Their values and derivation methods are outlined in Technical Support Documents (TSD) reviewed by the National Academy of Sciences (NAS) and are publicly accessible from the US Environmental Protection Agency's (USEPA) AEGL Chemical Data website.

i. Significance / Rationale

AEGL values are intended to be used in risk assessment, in the development of emergency preparedness and prevention plans, and in an actual response to an unforeseen chemical release. Their information of toxic endpoints at increasing exposure durations can be combined with chemical-release and dispersion models to identify geographical locations of high airborne exposures, vicinity to human populations and facilities, and estimate their risk of adverse health effects. This information is particularly important for emergency response personnel in making informed risk management and communication decisions to protect the general public. Such decisions include public notification and instruction, sheltering-in-place, evacuation procedures,

facilitation of medical attention, or a combination of these options (NAS 2001). In addition to protecting the public, AEGL exposure-duration data also protect emergency response personnel by providing information on how much time individuals can remain on-site before reaching an exposure concentration of adverse health concerns (e.g., irritation, disabling, or death).

The existing AEGL database is not comprehensive for all hazardous inhalation chemicals. Currently, less than 1% of commercially used compounds have AEGLs assigned. Only 329 compounds have been identified in the AEGL Chemical Priority Lists, from which 273 chemicals were selected for AEGL development. Among these, 42% (115) have unassigned AEGLs due to insufficient data or biological implausibility of estimates. These unassigned AEGLs are concentrated in the AEGL-1 threshold, which comprises of 91% (109) of all compounds with unassigned AEGLs. As of November 2011, AEGL development program will focus only on finalizing compounds with Interim AEGLs and will not review any new compounds. Therefore, a need for a rapid and cost-effective substitute for AEGL development is imminent.

The development of an efficient method to derive provisional AEGL values for compounds in the database with unassigned values or for new compounds will enable rapid risk assessment and emergency response to airborne hazard releases involving these compounds. In addition, such method would be useful in validating current AEGL derivation methods and complement data from in vivo toxicity and human epidemiological studies, which are often insufficient. In light of the administrative changes in the AEGL Program, these models can also be used to validate the consistency of the newly finalized AEGLs to previously developed AEGLs and flag for any systematic differences in the data.

ii. Specific Aims

The aim of this research is to develop an efficient statistical method for estimating AEGLs that align with experimental data and other existing HGVs for that compound. Employing correlation and linear regression analyses, the possibility of extrapolating AEGLs across at multiple exposure durations and health severity thresholds levels will be explored.

iii. Background/ Literature Review

A. Emergency response and the need for protecting the public

Hazardous substances can be released by industrial or transportation incidents, fires, severe weather, natural disaster events, terrorist attacks, or a human error. In effect, the nearby public and emergency response personnel are directly at risk of acute exposure that can lead to a range of adverse health effects (Krewski et al. 2004). In a chemical spill, the typical population size expected to be at risk in the United States ranges from 1,000 to 5,000 persons, depending on conditions of population density, concentration and rate of release, weather, climate, and the topography of the source site (NAS 2001). Hence, investment into emergency planning and response, public health risk assessment, and the development of protective HGVs are of high importance (Collar et al. 2011).

B. Protective Action Criteria (PAC)

Protective Action Criteria (PAC) for chemicals are guidelines used to plan and respond to hazardous chemical release incidents. For emergency planning, they are used to estimate health risks and establish priorities for prevention measures. For emergency response, PAC are used to assess the magnitude of exposure, identify possible health outcomes, and make important health protective decisions. PAC are derived from three existing acute exposure limit values: Acute Exposure Guideline Level (AEGL), Emergency Response Planning Guideline (ERPG), and

Temporary Emergency Exposure Limit (TEEL) (SCAPA 2010). These values all address three common health endpoints: (1) mild, reversible health effects, (2) irreversible or other adverse health effects that impair one's ability to take protective action, and (3) lethal health effects or death (SCAPA 2010). They are described below in more detail:

Acute Exposure Guideline Level (AEGLs): Established by the National Academy of Sciences (NAS) and the United States Environmental Protection Agency (USEPA), AEGLs represent levels "above which" health effects are expected and are developed for five exposure durations of 10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours. They are developed through a comprehensive peer-review process of primary toxicological information and are based off of a single key study. They are intended for protection of the general public including susceptible populations (SCAPA 2010).

Emergency Response Planning Guideline (ERPGs): Established by the American Industrial Hygiene Association (AIHA), ERPGs represent levels "below which" certain health effects are not expected and are developed for 1 hour exposure duration. Like AEGLs, ERPGs are derived for the protection of the public, are from a rigorous peer-review process of primary sources. Yet, they are based off a weight-of-evidence approach. Therefore, ERPGs are not routinely employed because of inconsistent methodology, insufficient data, and are for only one exposure duration (SCAPA 2010).

Temporary Emergency Exposure Limits (TEELs): Established by the Subcommittee on Consequence Assessment and Protective Actions (SCAPA), TEELs represent levels "below which" certain health effects are not expected and do not have specific exposure durations, although a 1 hour duration is implied. Although TEELs are published for over 2,500 chemicals, their derivation methods are less rigorous, from secondary sources, and often not explicitly stated. TEELs are constantly updated when different exposure limits

are published. Unlike AEGLs, TEELs are not derived for protection of the public but are more for emergency response personnel (SCAPA 2010).

C. AEGLs: Advantages and Disadvantages

The U.S. Department of Energy's (DOE) hierarchy for the selection of PAC is first AEGLs, then ERPGs, and lastly TEELs. AEGLs are one of the most internationally and frequently used respiratory HGVs and are preferable for several important distinctions:

- AEGLs encompass the most up-to-date and peer-reviewed PAC for inhalation exposures.
- Compared to ERPGs or TEELs, AEGLs are also intended to protect susceptible populations and have safety factors incorporated into their estimates (SCAPA 2011).
- AEGLs were developed for multiple exposure durations through the use of time-scaling extrapolations. In contrast, ERPGs are limited to the 1 hour contact time and are generally not recommended for extrapolation to other time points.
- The AEGL derivation process is more standardized and transparent (SCAPA 2010). AEGL values and their TSDs are publicly available data and comprise one of the largest databases for inhalation chemicals (NAS 2011).

In addition to the above differences, the discrepancy between AEGL and ERPG values can also be attributed to a different selection of critical effects, key studies, interpretation and evaluation of the data (Oberg et al, 2010). Therefore, based on their credibility, transparency, multiple exposure durations, and applicability for protection of the public in emergency scenarios, our study will focus only on AEGLs for statistical model development.

D. History of AEGL Development

The National Advisory Committee for the Development of Acute Exposure Guideline Levels for Hazardous Substances (AEGL/NAC) Committee was formed in 1986 after the Union Carbide

Limited (a subsidiary of the U.S.'s Union Carbide Corporation) industrial disaster in Bhopal, India in 1984. The goal of the committee was to develop AEGLs for hazardous chemicals for use in chemical emergency programs. These guidance values could then be used by federal, state, and local agencies, private sectors, and foreign organizations for emergency planning, prevention and response activities related to the accidental release of hazardous substances (NAS 2001).

In 1988, the USEPA's Office of Pollution Preventions and Toxics became interested in developing a method for creating short-term exposure guideline levels. In collaboration with ATSDR, they provided funding for a cooperative agreement with the NAS to develop such methods. The methodology, entitled "Guidelines for Developing Community Emergency Exposure Levels for Hazardous Substances," was published in 1993 and is based on a chemical approach. Subsequently, federal and state agencies and private sector organizations were contacted to form a joint committee that would focus on developing exposure guideline levels. Since then, they have identified 329 priority chemicals and have published AEGLs for 273 compounds to date. In November of 2011, the AEGL Committee officially ceased operation due to budget constraints. The AEGL Program remains active and collaborates with the National Academies to publish finalized AEGLs from those that are Interim in the existing database. For the time being, they will no longer be developing AEGLs for new compounds (NAS 2011).

E. Purpose and Definitions

AEGLs are short-term airborne threshold exposure limits developed to protect workers and the general public in the event of a hazardous chemical release. Concentration limits were developed for five durations (10 min, 30 min, 1 h, 4 h, and 8 h) at three severity thresholds of toxic effects (AEGL-1, AEGL-2, and AEGL-3). Airborne concentrations above each AEGL threshold indicate a progressive increase in the probability of the onset and severity of the corresponding health effects (Krewski et al. 2004). Thus, the three AEGL thresholds can be considered a dose-response curve and provide valuable insights into the estimated margin of safety between an exposure level

of mild irritation effects (AEGL-1) versus one that may disable one's ability to escape (AEGL-2) to death (AEGL-3) (Appendix 1). Higher exposure concentrations increase the likelihood of experiencing adverse health effects at the higher threshold. Although the recommended limits are for the general population, additional safety factors have been applied to account for sensitive populations such as infants, children, the elderly, and asthmatics (NAS 2001). Specific definitions for each AEGL threshold are below:

> **AEGL-1:** Level of airborne concentration above which individuals are predicted to experience notable sensory discomfort, irritation, or certain asymptomatic non-sensory effects. Effects are transient and not disabling or lethal (NAS 2001). Yet airborne concentrations *below* the AEGL-1 level can also produce mild and progressively increasing but transient symptoms (Krewski et al. 2004).
>
> **AEGL-2:** Level of airborne concentration above which individuals are predicted to experience irreversible or serious, long-term adverse health effects or an inability to escape. 'Inability to escape' is defined as an impairment requiring assistance and/or medical attention.
>
> **AEGL-3**: Level of airborne concentration above which individuals are predicted to experience life-threatening health effects or death.

F. AEGL Development process

1. Objectives:

Through a peer-review process of the Federal Advisory AEGL Committee and stakeholders, the AEGL development process has several aims: (1) development of scientifically valid AEGL values, (2) comprehensive identification of published and unpublished literature, (3) the exchange of resource burdens by stakeholders, and (4) the adoption of consistent emergency planning both domestically and overseas. In addition, the AEGL development committee aims for transparency of program methods through the publication of the Standard Operating Procedures (SOPs) and

inviting the public to participate in meetings and the commenting of Federal Register notices. Lastly, NAS is included in the peer review and decision-making process of AEGL methods and values to ensure scientific credibility.

2. Review process: AEGL stages

The process established for the development of the AEGL values is currently the most comprehensive for determining short-term exposure limits for acutely toxic chemicals. The process consists of four basic stages that represent review status of AEGL values: (1) Draft, (2) Proposed, (3) Interim, and (4) Final (Appendix 2).

Stage 1- Draft AEGLs: Published scientific literature and unpublished data from industry-trade associations and private companies for chemical are collected and evaluated following NAS' published guidelines in the SOP manual. Each chemical under review has its own AEGL development team, which is comprised of staff scientists at the organization, a chemical manager, and two chemical reviewers. They develop the TSD for draft AEGLs, which then undergo internal review by AEGL Committee members. A formal committee meeting is convened to present and discuss AEGL values and accompanying scientific documents. A quorum of at least 51% of the total AEGL Committee membership needs to be present.

For elevation of AEGL values to the "Proposed" status, a two-thirds majority vote is needed. If agreement is not reached, issues and concerns are raised for reassessment by the AEGL development team. After completion of reassessment, the chemical is resubmitted to the committee for a two-thirds vote. If consensus again cannot be reached due to insufficient data, AEGL values for the compound will not be developed until adequate data is available.

Stage 2- Proposed AEGLs: Proposed AEGLs are published in the Federal Register for a 30-day review and comment period. The AEGL committee resolves relevant issues from the comments.

The AEGL values and accompanying scientific rationale are then resubmitted for two-thirds majority vote. If passed, they then move to the "Interim" stage.

Stage 3- Interim AEGLs: AEGL values at this stage represent the best of the AEGL Committee's efforts to establish exposure limits. Values at this stage can be implemented by federal and state regulatory agencies and the private sector if deemed appropriate. Interim AEGLs, their supporting scientific rationale and TSD are presented to the NAS Subcommittee for review and concurrence. If agreement is reached, AEGLs are considered "Final" and published by the NAS. If not, they undergo review and revisions by contractors.

For any comments during this process that may result in changes to AEGL Interim values, the contractors would submit the revisions and TSD of the compound to federal stakeholders for a two-week review. The NAS then receives all revisions and will address these comments if there is lack of agreement between federal stakeholders. Interim AEGLs are then finalized with approval from NAS.

Stage 4- Final AEGLs: Final AEGLs may then be used on a permanent basis by all federal, state and local agencies, and private organizations. If new data become available that challenge their scientific credibility, the compound can be resubmitted for review through the same process outlined in the Interim stage.

3. AEGL derivation:

a. Data source:

Key toxicity studies and supporting data used for AEGL derivation are from electronic and government databases, peer-reviewed journals, published books and documents from the public and private sectors in the US and internationally, and data from private industries or organizations. Search criteria include references to toxicology, regulatory initiatives, and general

chemical information. AEGL derivation is solely based off of primary toxicology data of animal or human studies. Secondary sources can only be used for background information on chemicals not related to toxicology (Appendix 3).

For key toxicity studies, those focusing on the inhalation exposure route are preferred. If not available, oral exposure may be considered if systemic toxicity is the health endpoint of concern and hepatic fist-pass metabolism is not significant. For human data, the AEGL Committee relies on available clinical, epidemiologic, and case report studies that are in compliance with ethical standards and have publicly available, non-identifiable data. Clinical health effects data such as histopathologic changes, clinical chemistry, and hematology are included to reduce uncertainty. While studies of humans are most relevant, studies of animals like rats, mice, rabbits, guinea pigs, ferrets, dogs, or monkeys are acceptable. Consideration of other species requires further evaluation. Lastly, all relevant data should be evaluated and included in TSDs for a complete weight-of-evidence assessment of the available data. Additional criteria for AEGL data selection are outlined in the SOP document (NAS 2001).

b. Methods:

For the development of AEGLs, the Committee selects the health endpoint or point of departure (POD) reflecting the highest derived concentration without any observable symptoms or AEGL tier-specific health effects. This concentration represents the starting point for AEGL development. Three approaches exist for deriving AEGL values:

1. The first is based on experimental data of the No Observed Adverse Effect Level (NOAEL), defined as the highest experimental concentration at which there is no noticeable adverse health effect in an experiment where death was observed.
2. The second is by estimating the lethality threshold from one-third of the lethal concentration at which 50% of experimental species die (LC_{50}) to statistically obtain the 1% response (LC_{01}) value. A divisor value other than 3 can be used if more appropriate.

3. The third method is to use benchmark exposure calculations of the 1% and 5% response. Benchmark concentrations (BMC) are derived from mathematical and statistical modeling of experimental data points. The 1% to 5% response range is selected to approximate the lower limit of the adverse health effects that are likely to be observed in animal and human studies. Mathematical methods used in deriving benchmark concentration at the lower 1% response (BMC_{01}) are probit analysis and maximum likelihood estimates (CA EPA 1999) (Appendix 4). Additionally, the USEPA's log probit benchmark dose software can also be used for comparison (USEPA 2012).

The NOAEL approach is less credible because it is usually derived from only one experimental study, which can often be arbitrary and vary by the sample size of animals tested. The BMC approach is most preferable for selecting AEGL endpoints. It has strengths of (1) lower uncertainty than the NOAEL data, (2) the ability to estimate concentration when NOAELs are not established, and (3) the ability to use all experimental data to estimate dose-response curves when applicable (Grant et al. 2007).

c. Limitations of exposure-response extrapolations:

There are many uncertainties associated with exposure-response extrapolations. AEGL derivation for certain chemicals may not be appropriate or may have data limitations. The method that produces estimated AEGL values most consistent with the empirical data and the shape of the exposure-response curve are recommended. Estimated values that conflict with experimental values data are not used (NAS 2001).

For AEGL-1, due to the subjectivity of its health endpoint (e.g. sensory irritation, mild discomfort), its values may not be detectable at the AEGL-1 level or exceed that of AEGL-2s for certain chemicals. Also, there may be insufficient data available to establish AEGL-1. In such circumstances, AEGL-1 values for these chemicals are not established (NAS 2001). For AEGL-2, when there is a lack of specific data used to determine an AEGL-2 value, one third of the AEGL-

3 value has been used. This approach is valid only if there is a steep exposure-based relationship between data for effects below the AEGL-2 value and data of lethal-effects observed at the AEGL-3 value for that chemical.

AEGL-3's health endpoint of lethal effects or death is easier to observe. Thus, it faces less uncertainty in its derivations. Inhalation LC_{50} is most relevant and comparable to BMC analysis (NAS 2001).

d. Applying Uncertainty Factors (UFs):

To account for known and unknown variations in the toxicological response of organisms to chemical exposures and for extrapolations within and across species to human populations, uncertainty factors (UFs) are applied to experimental data. Determination of UFs is based on all available chemical data (e.g., its mechanism of action and structural analogues), weight of the evidence, toxicodynamic and toxicokinetic information, and informed professional judgment. Intraspecies UFs are incorporated to account for differences within species and address sensitive populations or those clinically compromised (e.g., women, children, or asthmatics). Interspecies UFs are incorporated to account for differences in extrapolation from animal to human data.

The POD experimental value is divided by the sum of all UFs to establish the appropriate AEGL value for specific health severity threshold and exposure duration. The magnitude of UF applied to account for interspecies and intraspecies variability is usually between a factor of 1 and 10. The UF selected is based on the robustness of the available data for a specific chemical. For susceptible populations, there is an additional UF between 3- and 10-fold applied derive AEGLs. Overall, the general guideline for which inter- and intraspecies UFs to use is 10 if there is an absence of adequate data and 3 or 1 if credible information is available (NAS 2001).

e. Additional Modifying Factors (MF):

Additional modifying factors of 2 or 3 can be applied to chemicals with (1) limited data, (2) health endpoints that were more severe than the AEGL-tier definition, and/or (3) variation in toxicity information between chemical isomers (NAS 2001).

f. Time scaling:

Often, toxicity data is not available for multiple exposure durations and must be extrapolated from Haber's rule and its ten Berge' modification. Haber's rule (1924) is:

$$C \times t = k$$

where C = exposure concentration
t = exposure duration
k = cumulative exposure constant.

The formula states that C and t can be reciprocally adjusted to obtain a cumulative exposure-response constant represented by k for that chemical. Haber's law is only applicable when the chemical response is equally dependent on C and t and where effects are irreversible and system repair is not expected. This law is generally not applicable to acutely toxic short-term exposures (NAS 2001; Gaylor 2000). Also, Haber's law will not apply to chemical toxicity relationships that are exponential, such as with most LC_{50} data.

Hence, there is a ten Berge modification to the Haber's law, $C^n \times t = k$, that accounts for compounds with varying dependence on C and t. The n exponent is the chemical-and toxicity-specific endpoint. A higher n indicates greater chemical-specific toxicity and in effect, yields a steeper decrease in the concentration-versus-time slope. Therefore, a n value above 1 indicates that the chemical's toxicity is primarily due to concentration rather than duration of exposure. An n value below 1 indicates the inverse--that the chemical's toxicity is more dependent on duration of exposure (CA EPA 1999). When n is equal to 1, the ten Berge modification is equivalent to Haber's law (NAS 2001).

The derivation of n is based on empirical data. If the data is insufficient, a default value of 1 or 3, representing the lower and upper boundary respectively, is selected. This range was estimated from a study by ten Berge et al (1986), which showed that extrapolations for 90% of the sampled chemicals had fell within this range. To derive the most conservative and health protective AEGL value, the n default value recommended for extrapolating from a shorter to a longer duration is 1. For extrapolations from a longer to a shorter durations, a n default value of 3 is recommended. The estimated AEGLs from these time-scaling methods are then cross-validated with supporting empirical data (NAS 2001) (Appendix 5).

g. Uncertainties in time-scaling and extrapolations of AEGLs across exposure durations:
Extrapolations across longer temporal ranges have greater uncertainty and require more supporting data and/or assumptions. Thus, extrapolations to the 10 min AEGL from a 4 h or 8 h POD empirical value are not recommended. Instead, the 30 min AEGL will often be used as the surrogate value for the 10 min value for that compound. Extrapolations to exposure durations below 10 min are not recommended because of the high data uncertainty at the acute exposure durations.

Time scaling applications to the lowest AEGL-1 threshold are more difficult and may not be appropriate due to the subjectivity of its health endpoint. The detection of discomfort such as odor or skin irritation is less recognizable and can vary between subjects as compared to the AEGL-3 endpoint of lethality or death. In addition, mild sensory effects like odor irritation may not be cumulative over time due to olfactory fatigue, adaptive responses, or a threshold effect of the compound. Therefore, AEGL-1's health effect may be independent of exposure duration and thus, time-scaling extrapolations would be inappropriate for these compounds (NAS 2001).

iv. AEGL applications in public health

A. Aims of AEGL program

The main purpose of the AEGL committee and AEGL development were to establish health protective action criteria for acute airborne exposures to hazardous, high-priority substances. These criteria could then be applied towards planning, response, and prevention initiatives. Existing federal initiatives in which AEGLs can be applied are the USEPA's Superfund Amendments and Reauthorization Act emergency planning program, the Clean Air Act Amendments accident prevention program, the remediation of Superfund sites program, the DOE's environmental restoration, waste management/transport, and fixed facility programs, and the ATSDR's health consultation and risk assessment programs. In addition to federal programs, AEGLs can be applied towards international emergency planning and response programs (NAS 2001).

B. AEGLs and geospatial modeling

AEGLs have also been used in the geospatial modeling of public safety zones in event of a toxic release (O'Mahoney et al. 2008). This risk assessment approach employs AEGLs at the 10 minutes and the Areal Location of Hazardous Atmospheres (ALOHA) modeling software to determine populations at risk based on their distance to the source. The aim is to create an emergency plan in which responders can rapidly identify populations at risk and triage them by levels of toxicity concern. Hence, the three modeled dispersion plumes of "hot", "warm", and "cold" zones represent AEGL -1s, -2s, and -3 health endpoints, respectively (Appendix 6). The "hot" zone characterizes individuals exposed to concentrations above the 10 min AEGL-3 severity threshold, who are at risk of life-threatening effects and would be higher in priority for medical attention and/or evacuation. The "warm" zone characterize individuals exposed to concentrations above the 10 min AEGL-2 threshold, who are at risk of non-lethal but irreversible effects and should be monitored long-term. The "cold" zone characterize individuals exposed to

concentrations above the 10-min AEGL-1 threshold who may not exhibit immediate symptoms but may experience discomfort and irritation (O'Mahoney et al. 2008).

C. AEGL comparability to existing HGVs

Databases of several exposure limits for hazardous compounds vary in their target populations, definitional aims, exposure duration, health endpoints, and methods of data extraction. Two frequently referenced exposure limits of airborne toxicants are the U.S. National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limits (RELs) and the American Conference of Government and Industrial Hygienists (ACGIH) Threshold Limit Values (TLVs). RELs are peer-reviewed maximum airborne exposure concentrations for workplace hazards that should be preventative of adverse health effects like cancer (NIOSH 2012). These recommendations are published and sent to the Occupational Safety and Health Administration (OSHA) and Mine Safety and Health Administration (MSHA) for use in the development of enforceable standards. ACGIH's TLVs are developed by a private organization and updated yearly for compounds of airborne exposures. By definition, TLVs are airborne concentrations below which the majority of workers, when daily and chronically exposed over a working lifetime of 40 years, will not experience adverse health effects (ACGIH 2007).

Both RELs and TLVs are occupational exposure limits (OELs) developed for the average U.S. working adult for a chronic lifetime exposure scenario. The limits are characterized by two types of values: time-weighted averages (TWAs) and short term exposure limits (STELs). TWAs are the time-weighted average concentration for a work-day during a 40 hour work week. Specifically, REL-TWAs are for a 10 hour work day whereas TLV-TWAs are for an 8 hour work day. STELs are developed for compounds in which adverse effects at the acute workplace exposure durations of 15 minutes are expected in addition to chronic exposures. According to both NIOSH and ACGIH, a STEL value should not be exceeded at any time during the work day. It represents the concentration below which workers can be continuously exposed in a short

period of time without experiencing irritation, chronic or irreversible tissue damage, dose-rate-dependent toxicity, or unconsciousness that increases individuals' susceptibility to injury and impairs his/her ability to escape or perform work efficiently (ACGIH 2007).

In contrast to RELs and TLVs, AEGLs are health threshold levels developed for the protection of the general public, including susceptible individuals. Each threshold represents a specific adverse health endpoint at five short-term exposure durations. Additionally, AEGLs were developed for acute once-in-a-lifetime or rare exposures scenarios such as a chemical spill. They are derived from acute toxicity data instead of sub-chronic and chronic studies like for RELs and TLVs. Despite discrepancies between comparing OELs and AEGLs, it is likely that AEGLs at the lowest severity threshold of sensory irritation (AEGL-1) would be most similar to OELs, and that AEGLs at the shorter exposure durations would be more similar to STELs. Yet, the relationship between acute and chronic exposure values needs to be explored. A method for their comparison is presented in the present study.

II. METHODS

i. Hypothesis

The hypothesis of our study is that statistically credible models can be developed to predict provisional AEGLs for compounds with unassigned values, based on the underlying relationship of the AEGL database. We hypothesized that higher correlations will be observed between AEGLs at closer severity threshold levels and exposure durations due to similarities in the physical-chemical characteristics of inhalable compounds and uniformity of procedures by which the AEGLs have been developed. All compounds in the AEGL database are for acute, inhalable airborne exposures. Also, the procedures for the selection of key studies, application of uncertainty factors, and extrapolation from POD values across exposure durations and severity thresholds should be standardized to SOP guidelines. Therefore, we expect our models to reflect the underlying correlational and linear relationship of the AEGL database and that the "best" predictive models will encompass AEGL parameters with the best fit.

ii. Methods of data collection

A. Data source

Information about key studies and supporting scientific documents for each compound in the AEGL database is published in USEPA's TSD and publicly available on their AEGL Chemical Data website (http://www.epa.gov/oppt/aegl/). TSDs contain the methodological information, scientific rationale for time scaling and uncertainty factors, chemical toxicity, and a table of AEGL values with their respective rationale and references for the AEGL derivation (NAS 2001).

B. Data extraction

Qualitative and quantitative data for all Final, Interim, and Proposed compounds in the USEPA's AEGL database were extracted from their respective TSDs. For example, to retrieve the TSD for aniline, one would go to the USEPA AEGL Chemical Data website, select the "AEGL

Chemicals" hyperlink, and search for aniline by its Chemical Abstracts Service (CAS) numbers or chemical name. In a new window, the AEGL values for aniline will appear and its respective TSD is provided in the hyperlink "Technical Support Document." Compounds in the Draft AEGL stage were not extracted for analysis. Two methods for data extraction from TSDs were used and cross-referenced: A Linux programming code and manual search. Databases with relevant information were constructed in Microsoft Office 2010 Excel (Redmond, Washington) and JMP 9.0.2 (SAS Institute, Cary, NC) statistical software.

Quantitative data collected for each chemical were:

1. AEGL reported values (continuous or NR for 'Not Recommended')
2. Molecular weight (g/mol)
3. Time scaling factors : C (ppm), t (hour), k (ppm·h), and n (a constant)
4. Uncertainty factors applied (intraspecies and interspecies)
5. Modification factors applied

Qualitative data collected for each chemical were:

1. USEPA AEGL development stage (Final, Interim, or Proposed)
2. CAS number
3. Published concentration value (in parts per million (ppm) or milligrams per cubic meter (mg/m^3)
4. Key study used
5. Toxicity endpoint or point of departure value and its exposure duration

C. Data validation:

The Simplified Molecular Input Line Entry System (SMILES) containing structural notation for each chemical were previously derived in-house and updated from the ChemIDplus Advanced (US National Library of Medicine). The 2010 ChemOffice Ultra 12.0 software (Cambridgesoft) was used to extract and verify chemical properties and structural data such as SMILES, and molecular weight.

D. Data cleaning and conversions:

AEGL values are based on a standard temperature and pressure assumptions of 25°C (299 K) and 760 mm Hg, respectively. AEGL concentrations reported in parts per million (ppm) in TSDs were

derived using a volume-by-volume approach. Those reported in milligrams per cubic meter (mg/m^3) were derived by a mass-by-volume approach and are susceptible to external factors such as pressure, volume, and/or temperature and variability at different elevations above sea level. At least 41 of the compounds in the USEPA's database were reported in mg/m^3. These compounds were converted to ppm for consistency of the AEGL database. Calculations for the unit conversion are in Appendix 12.

iii. Methods of analysis

A. Descriptive statistics of the AEGL database

1. Test of normality and frequency of unassigned values

Descriptive analysis of the AEGL dataset was conducted using SAS' PROC CONTENTS and PROC UNIVARIATE functions. Information of sample mean, standard deviation, median, and interquartile range were obtained. Additionally, skewness, histograms, and the normal probability plots were evaluated for normality. If the data failed the normality assumption, $\log_{10}$ transformation was applied to the database and used for all analyses. The frequency and pattern of unassigned AEGLs were also assessed in JMP.

2. Pearson correlation analysis

Pearson correlations coefficients measured the degree of linear co-relation between two normally distributed AEGL pairs (Rigby 2008). A fifteen-by-fifteen Pearson correlation matrix was constructed for all AEGLs-1,-2, and -3 at five exposure durations (10 min to 8 h) in JMP. For each duration-and-threshold-specific AEGL level, 15 different Pearson correlation coefficients (r) were derived, representing the linear relationship between itself ($r = 1$) and the 14 unique duration-and-threshold-specific AEGL levels ($0 < r < 1$). In total, correlation matrix contained 225 coefficients, from which 105 were unique pairs. Depending upon frequency of unassigned

values, each level can have up to 273 AEGL data points representing different compounds. The magnitude of *r* represents the proximity of the data points to the line (Twomey and Kroll 2008).

B. Model building

1. Deming Linear Regression

Deming linear regression (DLR) was employed in the present study to assess the linear dependence of each duration-and-threshold-specific AEGL level to one another. DLR simultaneously minimizes the distance of data points orthogonally to the regression line in both the x and y-axis. As a result, only one regression line is produced (Linnet 1993; Helsel and Hirsch 2002). In contrast, the more common ordinary least-squares regression (OLR) assumes that random error measurements exist only in the y-axis and that the x-axis data is error-free. Therefore, two regression lines can be produced depending on which axis is selected as referent (error-free) (Linnet, 1998) (Appendix 7). Since the aim of the study was to develop predictive models from AEGL pairs, the DLR method producing one regression line is preferred. It accounts for potential variability in AEGL values between duration-and-severity threshold-specific levels. These sources of variability can be attributed to the use of different key studies across severity thresholds and the use of different time-scaling factors for extrapolations across exposure duration in AEGL derivation. Though, the variance ratio was assumed to be 1 for all levels (λ=1) (Tan and Iglewicz 1999).

2. Deming linear regression procedure SAS Macro

The SAS® Macro for Deming Regression (Deal et al. 2011) was used for DLR analysis of the 105 unique duration-and-threshold-specific AEGL pairs. The macro was chosen because DLR analysis was not an available in SAS 9.3 (Cary, North Carolina) and JMP's orthogonal regression function did not produce CIs of the y-intercepts (Linnet 1998; Tan and Iglewitc 1999). To obtain Deming regression estimates of slope, intercept, their standard errors (SEs) and 95% CIs for each

of the 105 duration-and-threshold specific models, Linnet's (1998) DLR equation was applied with λ =1 (Appendix 11).

$$Y_{esti} = a + b(x_{esti} - x_m) = a_o + bX_{esti} \quad \text{(Eq. 1)}$$

where:

Y_{esti} = $\log_{10}$(Response AEGL value at specific exposure duration and threshold)
X_{esti} = $\log_{10}$(Predictor AEGL value at specific exposure duration and threshold)
a = $\log_{10}$(y-intercept) = $\frac{\sum y_i}{N}$ = sums of squared deviations in the y estimate, its SE are estimated from resampling procedures
b = coefficient of X_{esti}, its SE are estimated from resampling procedures
x_m = $\frac{\sum x_i}{N}$ sums of squared deviations in the x estimate
a_o = $a-b \cdot x_m$

The Deming macro is a series of multiple DATA steps and PROC MEANS statements to calculate the slope and intercept of the Deming regression. Non-parametric, leave-one-out Jackknife resampling methods and a Student's *t*-distribution with *n*-1 degrees of freedom were used to derive standard errors and construct CIs for the slopes and intercepts. The sample size (n) for each level was the number of assigned AEGLs available.

3. Bootstrap resampling of the 95% prediction intervals for the DLR fit

a. Differences between CI and PI

A prediction interval (PI) is defined as the interval that contains the values of a specific number of future observations at a specified probability, for which a single observation is expected to fall within the interval (Hahn 1969). Confidence intervals (CI) estimate the distribution around the true population parameter such as the regression line. PIs are general wider than the CI because it accounts for the variability of the single data point around the regression line and the error in its estimate to the center of the distribution (Helsel and Hirsch 2002). Since the aim of the present study was to develop statistical models to predict provisional AEGLs, analysis of PIs instead of CIs was most appropriate.

b. Bootstrap resampling methods

DLR 95% PIs that accounted for the variability and errors for both the slope and y-intercept estimates were needed. To construct these 95% PIs, a novel code was developed by a colleague, Yunfeng Tie, from ATSDR/DTHHS/ETB, that to the author's knowledge has not been presented elsewhere. The code was developed in R software (www.r-project.org/) and based on Davison and Hinkley (1997)'s prediction interval equations Appendix 13. Overall, the bootstrapping method for the 95% prediction intervals of the Deming regression consisted of repeated random resampling with replacement, in which each observation has the equal probability (1/n) of being resampled. The equation was reiterated 1000 times to get percentile estimates for each parameter. The PI percentile estimates were ranked in order of magnitude and the 2.5% and 97.5% percentiles were selected as limits for the 95% PIs. Bootstrapping is a useful method to generate more robust, non-parametric estimates of the confidence or prediction intervals when the underlying distributions are non-normal or potentially non-linear (Efron and Tibshirani 1993).

C. Model analysis

1. Test of statistical identity of regression coefficients

Statistical identity of the regression estimates for each AEGL pair was assessed by testing the Deming regression coefficients of the Deming slopes (b) and y-intercepts (a_0) for a significant difference from the null value of 1 and 0, respectively (Tan and Iglewicz 1999). The Deming Jackknife 95% confidence intervals of the estimated slopes and intercepts for each model were used to assess for statistical identity. A model with a slope significantly different from 1 (its 95% CI_{slope} does not contain 1) suggests that the two data vary by a proportional amount, or is multiplicative on the log-scale. A model with an intercept significantly different from 0 (its 95% $CI_{y\text{-}intercept}$ does not contain 0) suggests that the two data vary by a constant amount, or is additive on the log-scale (MedCalc 2012). The aim of our study is to obtain non-significant slope, which

would suggests that the AEGL levels statistically similar and comparable (Tan and Iglewicz 1999).

2. Linearity

Twomey and Kroll's (2008) model analyses approach served as a guideline for our approach to analyze and select the best predictive models. Linearity of the AEGL models was graphically assessed by shape of the regression line, scatteredness of its data points, and residual plots of the predicted and observed values ($y = y_i - y_{bar}$) against their independent predictors (x). Homoscedasticity of points about the x-axis line at y=0 indicates that linearity of the model exists (Twomey and Kroll 2008).

3. Frequency of identical surrogate values

Identical surrogate AEGL values were often used within a threshold for the 10 min, 30 min, or 8 h exposure durations when there is uncertainty of time-scaling to the lowest of highest exposure durations based on ten Berge's modifications. The presence of identical surrogate values within a threshold may increase *r* values models with greatest prevalence of these values and bias model predictions. Thus, the frequency of identical surrogate values in each duration-and-threshold-specific level was evaluated for its influence on model performance.

D. Model Selection

1. Identifying the "best predictive" DLR models

The evaluation of the best predictive DLR models for each duration-and-threshold-specific AEGL level incorporated all of the above statistical analyses of correlations, residuals, PI width, and magnitude difference of estimates. For each AEGL response level, its correlation coefficients with the 14 other levels were ranked in order of highest to lowest. Similarly, DLR models of AEGL pairs were ranked by the width of their 95% PIs. AEGL pairs with the highest, middle, and

lowest rankings based on *r* and PI width, independently, were selected for preliminary analyses of their AEGL estimates. Rankings based on Pearson correlations were compared to those based on PI width for model selection consistency. If the rankings matched on both *r* and PI width, only one model was proposed. If there were discrepancies between models selected by *r* and PI width analyses, both models were selected for preliminary comparisons.

2. Assessment of model performance

The highest ranked DLR models based on *r* and PI width rankings were applied to compounds with already assigned AEGLs to assess their model performance. Model performance was characterized by the magnitude of difference between actual and estimated AEGLs and their residual plots. The three levels of magnitude difference (non-log) were by a factor of 3, -10, and -100. These cut-off range were selected to reflect the magnitude of uncertainty factors (e.g., for interspecies, intraspecies, time-scaling, and/or data extrapolations) that are generally applied to derive AEGLs. The percentage of compounds falling within each level was compared across selected models. Models for which a greater percentage of its AEGL estimates were within the lowest factor of 3 were selected as "best" models.

E. Model applications to derive unassigned AEGLs

The best predictive DLR models were then applied to compounds with unassigned values to estimate their AEGLs. Model selection considered first, (1) the width of their 95% PI, (2) residuals of their estimates, and lastly (3) their magnitude of Pearson correlation. Additional models were proposed, within and across severity thresholds, in the event that the highest predictor AEGL value was unassigned for that compound. The majority of compounds with unassigned AEGLs in the database existed predominantly in the AEGL-1 severity threshold. Therefore, models that encompass AEGL pairs from the same AEGL-1 threshold were not

developed, i.e. if an AEGL-1 at 10 minutes were unassigned, it is often the case that the AEGL-1s at all other durations were also unassigned.

F. External cross-validation of provisional AEGL estimates with existing HGVs

1. Data comparability of HGVs: OELs and AEGLs

For external cross-validation of AEGL estimates with other HGV data for air contaminants, a database of the occupational exposure limits (OEL), NIOSH's RELs and ACGIH's TLVs of both STELs and TWAs, was constructed for analyses of compounds overlapping with the AEGL database. DLR was employed in JMP to compare OELs to each other and to AEGLs. For OEL comparisons with the AEGL database, the STELs and TWAs of NIOSH's RELs and ACGIH's TLVs were regressed against each duration-and-threshold specific AEGL. These regressions were performed to derive 60 sets of DLR slopes, intercepts, correlations, and the 95% CIs of the slopes. Statistical identity of the slopes were evaluated ($\alpha = 0.05$) under the null hypothesis of slope = 1. The correlation for each regression model was ranked to identify the best fit models. Since we are only interested in assessing data comparability and not predictions between OELs and AEGLs, the 95% PIs of their regression line were not constructed.

2. Comparison of estimated AEGLs with OELs

Deming regression pairs of an OEL and a duration-and-threshold specific AEGL level that have higher correlations were assumed to be more similar. These AEGL-OEL pairs were then selected for external comparisons of compound-specific AEGL estimates at their respective exposure durations. The established "best" predictive models were then used to derive estimates for the AEGL levels that corresponded with the most highly correlated with OELs. Statistical identity of the AEGL estimates and their respective OELs was compared. Statistical identity was suggested if the OEL value fell within the 95% PI of the AEGL estimate for that compound.

III. RESULTS:

i. Descriptive statistics of the AEGL database

A. *Frequency of unassigned values*

The USEPA's AEGL database updated in November 2011 included 273 inhalable compounds. Stratified by their development status, 74 were Finalized, 187 Interim, and 12 Proposed (Table 1). Not all compounds had its full 15 AEGL duration-and-threshold specific values assigned. Of the 273, 115 (42%) had at least two unassigned AEGLs, from which 109 (94.7%) were concentrated in the AEGL-1 threshold. Only 6 (5.2%) compounds in the AEGL-2 threshold and 10 compounds in the AEGL-3 threshold had unassigned AEGLs (Figure 1). One compound, Nitric Oxide, although listed as Interim, did not have any AEGL values assigned. Unassigned AEGL values are reported as either "Not Recommended (NR)" or "Not Determined (ND)" in the USEPA's AEGL database, but were classified as NR to indicate both in our database. For the TSDs, the most commonly identified rationale for unassigned AEGLs were:

- Insufficient or inappropriate data for target health endpoint.
- Little margin between exposures of no effects and lethal exposures.
- Estimates were not biological relevant, exceeded odor threshold, and/or exceeded AEGL-2 threshold values.

B. Test of normality

The distribution of AEGLs at each exposure duration and severity threshold did not satisfy the normality assumptions. Skewness statistics for each level were much greater than the cut-off value of 0. Evaluation of their histograms and normal probability plots also showed a skewed right-tailed distribution. Log_{10} transformation of the AEGL data produced a log-normal distribution that could be fitted to a linear regression line, which was desirable for our DLR

analyses (Table 2). A log-normal model has been used in other HGV benchmark studies and shown to be biologically plausible (Collins et al. 2004).

C. Pearson correlation analysis

Pairwise correlations of log-AEGLs by their duration-and-threshold specific levels produced correlation coefficients (*r)* greater than 0.88. The highest correlations coefficients were observed for within threshold pairs, for cross-threshold pairs closer in exposure durations, and for cross-extrapolations between AEGL-2s and -3s instead of with AEGL-1s. Poor correlations were observed for all cross-threshold pairs at the 10 min exposure durations (Table 3).

ii. Model building

A. Deming linear regression

For each duration-and-threshold-specific AEGL level, there were up to 14 possible Deming univariate-linear regression models for a total of 210 models (Figure 2). Yet since DLR produces the one regression line for each X and Y regressed pair, our analyses was interested in only the 105 unique DLR models (Table 4).

iii. Model analysis

A. Test of statistical identity of regression coefficients

Assessment of the 105 models for statistical identity of the slopes and intercepts at the 95% probability resulted in 30 models (28.5%) with non-significant slopes, among which two (0.02%) had non-significant y-intercepts. Analyses of cross-threshold models show statistical identity among AEGL-1s regressed upon AEGL-2s at 4 h and 8 h, and AEGL-3s regressed on AEGL-2s at 10min and 30min durations (Table 4 and 5). Within threshold comparisons shows statistical identity in slopes for shorter exposures duration.

Slopes of for the remaining 75 (72%) models, although not statistically identical, were meaningfully similar to a slope of 1 and intercept of 0. For these models, the mean slope was 1.05 (min: 0.90, max:1.23) and the mean SE was 0.02 on the $\log_{10}$-scale. In contrast, almost all of the models had significantly different y-intercepts at the 95% probability, with an absolute mean intercept of 0.99 (min:-2.59, max: 1.23) and a mean SE of 0.04 on the $\log_{10}$-scale for the 105 models (Table 5). Further analysis is needed to understand the variations in statistical identity of the slopes and intercepts between models. Also, verification of SAS Macro's Deming estimates with those from JMP orthogonal and R's Deming bootstrapping code showed consistency of methods.

B. Linearity

Visual analysis of models from Figure 2 shows high linearity for all 105 models and characterizes the log-normal distribution of the AEGLs. Scatteredness of the data points about the y=0 line in their residual plots also suggest linearity (Figure 3). The residual plots also indicated that models with higher Pearson correlation and narrow prediction intervals had better linearity and a more uniform distribution of the SDs than models with lower *r* and wider PI widths.

C. Frequency of identical surrogate values

Analyses of the frequency of identical surrogates for each level showed that the AEGL-1 threshold had the highest count of identical values for at least 115 of the compounds (Table 6). There were less surrogate values present in the AEGL-2 (range:19 – 64 compounds) and AEGL-3 (range: 10 – 57 compounds). The observed higher frequency in the AEGL-1 threshold most likely reflects the lack of available data for acute exposure durations at the AEGL-1 health endpoint.

iv. Model Selection

A. Identifying "best predictive" DLR model

From model rankings based on correlation magnitudes, 45 unique duration-and-threshold-specific AEGL models were selected (i.e. 15 highest, 15 middle, and 15 lowest correlated models). Generally, models with higher Pearson correlations corresponded with those having narrower 95% PIs. Yet, their comparisons with models ranked by the 95% PI width showed that among the 15 models with the narrowest PI intervals, six of them did not correspond to models with the highest Pearson correlations (Table 7). Since models with narrower 95% PIs have more data points distributed closer about regression line, they are expected to have higher predictive potential than models with wider 95% PIs. Therefore, these six models were included for preliminary model performance analyses.

B. Assessment of model performance

Comparison of residual plots for high, middle, and lowest correlated DLR models for each duration-and-threshold-specific AEGL level supported earlier trends: models with poorly correlated data (yellow) had more scattered observations and less linearity than models with the highest correlated data (blue). Data points for these higher correlated models seemed normally distributed along the horizontal slope (Figure 3).

Comparison of percent coverage of estimates falling within a factor of 3-difference for all 51 selected models resulted in all of them having moderate predictions: at least 50% of compounds with estimates under 10 factors difference from actual values. Though, models that had the highest correlations and/or narrowest PI models had the highest percentages of estimates were within a 3-fold difference. Highest correlated models had 48-88% compound coverage compared to models that had mid-range (31%-75%) or the lowest correlations (31%-62%). In addition, the six models with the narrowest 95% PI width had the greatest coverage of

compounds within a factor of 3 (75% - 95%) (Table 5, Figure 4), suggesting that the PI width may be a more sensitive indicator of model performance.

v. Model applications to derive unassigned AEGLs

For each duration-and-threshold-specific AEGL level, the best predictive model was selected based on the width of their 95% PI, residuals of their estimates, and level of correlation, for a total of fifteen best models. In addition, two alternative AEGL pair models were proposed if the primary AEGL predictor were unassigned for that compound. Also, since the majority of unassigned AEGLs were in the AEGL-1 threshold, AEGL-1 predictors for an AEGL-1 level response were not presented (Table 8).

vi. External cross-validation of provisional AEGL estimates with existing HGVs

A. Data comparability of HGVs: OELs and AEGLs

NIOSH 2004's REL-TWAs and -STELs, ACGIH's 2007 TLV-TWAs and -STELs, and the AEGL database had at least 44 compounds that overlapped in all three databases (Table 9). Among these, 14 compounds had *unassigned* AEGLs within the AEGL-1 threshold. Deming regression of the occupational exposure limits (OELs) with each other showed that ACGIH's STELs and TWAs had a statistically significant slope, which suggests that they differ by proportional constant. All other OEL comparisons were statistically non-significant (Table 9).

B. Comparison of estimated AEGLs with OELs

Deming linear regression of STELs to assigned AEGLs indicated statistical similarity and had the highest correlations between ACGIH's STELs and AEGL-1 and -2 at the 4 h and 8 h exposure durations. Similarly TWAs were statistically similar and most correlated with AEGL-1 and -2 at the 4 h and 8 h exposure durations for both ACGIH's TLVs and NIOSH's RELs (Table 10).

For the 14 overlapping AEGL and OEL compounds the in database, with AEGLs unassigned for at least one threshold, their best model estimates for AEGL-1 and -2s at 4 h and 8 h were cross-validated with their ACGIH TLV-STELs, –TWAs, and NIOSH's REL-TWAs. NIOSH and ACGIH's TWAs were statistically indistinguishable (contained within the 95% PI) from AEGL-1, 4h and 8h estimates for 8/14 compounds. The ACGIH's STELs were statistically indistinguishable from AEGL-1 at 4h for 3/14 compounds. Internal validation of actual to estimate AEGL-2 values showed statistical identity for 10/14 compounds (Table 11).

IV. DISCUSSION

The objective of the present research was to develop an efficient statistical method to derive provisional AEGL values for inhalable hazardous compounds with unassigned values. The need for such a method in acute inhalation exposure risk assessment is high, due to insufficiency of toxicology and human data for adequate assessment of short term inhalation exposures. Within the AEGL database, 42% of the compounds in its databases have unassigned values. Additionally as of November 2011, the AEGL/NAC was disbanded from future work on AEGLs due to budget constraints and the AEGL Program will no longer review new compounds.

The present work proposes a statistical model that characterizes the relationship of the underlying AEGL database and that can be used to extrapolate statistically valid AEGL estimates across exposure durations and health severity thresholds. Such method is thought plausible based on the homogeneity of the existing database for inhalable compounds, standardized AEGL derivation methods to SOP guidelines, and an extensive peer-reviewed process by AEGL committee and external stakeholders before AEGLs are finalized. Employing Pearson correlation and Deming linear regression techniques, the statistical model provides a simple but promising approach to the statistical analysis and predictive inferences of HGVs of acute inhalation exposures.

The observed high Pearson correlations between duration-and-threshold specific $\log_{10}$AEGL levels, especially among those closer in exposure duration and health endpoints, suggest a log-linear association between all AEGL levels from which regression analysis can be applied. Correlation analysis has used other studies to comparison of acute reference exposures (Woodall 2005). Yet, the method is limited and does not provide information of the level of agreement between the AEGL pair, such as proportional or constant differences (Twomey and Kroll 2008). For example, a correlation of 1 could be observed between two levels even if AEGL-2 at 4 h were twice the magnitude of AEGL-1 at 1 h.

Therefore, the additional Deming linear regression analysis was performed in the present research as a better approach for evaluating the linear relationship between AEGL levels (Rigby 2008). DLR minimizes the distance of both AEGL level estimates orthogonal to the regression line and produces slope and y-intercept coefficients for each AEGL pair (Twomey and Kroll 2008). The DLR regression model parameters derived from compounds with assigned AEGLs were then used to extrapolate estimates for compounds with unassigned AEGLs in the duration-and-threshold-specific AEGL level of interest. Also, DLR was preferred over traditional regression techniques because it accounted for the likely uncertainty in the development of AEGL values across exposure duration and severity thresholds. Often compounds are evaluated on a case-by-case basis and their AEGL values reflect the weight-of-the-evidence, physiochemical characteristics, and AEGL Committee's recommendations for that compound.

DLR analyses of the log-transformed AEGL database showed strong linear relationships between the 105 unique duration-and-threshold-specific AEGL pairs. The discrepancy in statistical identity ($\alpha = 0.05$) of the slope and intercepts among the 105 models could be attributed to other parameters associated with AEGL values and/or their derivation that were not controlled for by the univariate model. It was thought that the frequency of identical surrogates AEGLs may be an indicator, but preliminary descriptive analyses suggested otherwise. Yet, the slopes of all models were meaningfully close to 1, despite not achieving statistical significance at the 95% confidence level. Interpretation of the slope and intercept for statistical identity is often limited. It does not provide information of the exact linear relationship and can only quantify the spread of the data about the regression line (Twomey and Kroll, 2008). Even with a slope of 1 and intercept of 0, datasets can have little agreement. Therefore, analysis of individual samples is preferred.

The present work applied several approaches to mathematically compare individual estimates produced by the DLR models. Non-parametric bootstrapping was employed to obtain the slopes, intercepts, their standard errors, 95% confidence and prediction intervals ($\alpha = 0.05$) and ensure validity of our models (Twomey and Kroll 2008). Our prediction intervals for DLR

were novel because they accounted for both errors in the slopes and intercept of the regression line. To the author's knowledge, no other study has employed such prediction intervals for Deming linear regression analysis. A narrower 95% prediction interval about the regression line is desirable and indicates that future AEGL estimates from the model will have 95% likelihood of being from the same the interval (Armstrong and Collopy 2001). DLR models with the narrowest PIs in our study corresponded with AEGL estimates closer in magnitudes to actual AEGL values. A positive relationship between Pearson correlation coefficients and width of PIs was observed across models but was not further explored in the current study. Residual analysis also showed that models with narrow PIs were also more log-linear, log-normal, and less scattered about the y=0 axis (Rigby 2008).

Our mathematical comparisons provided a systematic approach to estimate each models' predictive performance in order to select the "best" model for each duration-and-threshold specific AEGL level. We found that model performance was dependent on the exposure duration and severity threshold of its AEGL predictor and response levels. The best models were those with AEGL pairs closer in exposure duration and/or severity thresholds. They were characterized by the narrowest PI, highest percentage of estimates within a 3-factor difference of actual values, better residuals, and a comparatively high *r* value. By threshold, the best models for extrapolations to AEGL-1s were those regressed with AEGL-2s. For AEGL-2s extrapolations, models with AEGL-3s at the adjacent upper exposure duration were generally the best. Extrapolations for AEGL-3s were similar; the best models were with AEGL-2 at the upper adjacent exposure durations. Models with AEGL-1s as predictors yield a AEGL estimates greater than three-fold difference for the majority of compounds. Poorly predictive models were also found in the lower exposure durations of 10 min and 30 min for both AEGL-1s and AEGL-3s. The observed poor predictions are likely attributed to insufficient data and a smaller sample size within that AEGL level.

In the study, OELs were used as comparison values for assessing external validity of model predictions for unassigned AEGLs. Yet, this approach has recognizable limitations: OELs are maximum airborne exposure limits below which adverse health effects are not expected, intended for the average US working population, and characterize daily chronic exposures. In contrast, AEGLs are threshold limit values intended for protection of the general public in an emergency response and characterize once-in-a-lifetime acute exposures (Woodall 2005). Despite these differences, a previous comparison of OELs with acute reference exposures (AREs), inclusive of AEGLs, for a subset of compounds showed comparable estimates of OELs to AEGL-2s for inhalable compounds like acrolein and phosgene. The study suggests that OELs can serve as a useful fence line mark to assess allowable limits for AREs (Woodall 2005). Additionally, the health endpoint characterized for TLV-STELs (e.g., irritation, chronic to irreversible tissue damage, and disabling effects like narcosis) are similar to those of AEGL-1 and -2 thresholds. This suggests that TLV-STELs for a 15 min exposure may be most similar to AEGL-2 values.

The relationship was observed in Deming linear regressions of OELs to AEGLs at each duration-and-threshold-specific level. Statistical identity of the slopes at the 95% confidence level existed for all duration-and-threshold specific AEGL to OEL comparisons. The highest correlations were found between REL-TWAs, TLV-TWAs, and TLV-STELs, individually, with AEGL-2s at the 8 h and 4 h exposure durations. Subsequently, the next highest correlations were with AEGL-1s at the 8 h and 4 h exposure durations. The best model parameters were then applied to estimate AEGL-1 values for the 14 test compounds with unassigned AEGL-1s. Comparison of AEGL model estimates for the 14 compounds with their respective OELs showed statistical identity of AEGL-1 and OELs for 57% of compounds and 64% for AEGL-2s. Statistical identity refers to OEL values falling within the 95% PI of the estimated AEGL for the compound. Specifically for the compound phosgene, we observed statistical identity of its REL and TLV-TWAs with the AEGL-2 estimate at 4 h. This finding was similar to that of Woodall's

(2005), who compared the duration and severity of health effect multiple HGVs of phosgene and observed concentration similarity between the TLV and AEGL-2 at 4 h values (Appendix 10).

Overall, the univariate Deming linear regression models provides a statistical approach for estimating AEGL values, based on the underlying linear correlation of exposure durations and severity thresholds present in the AEGL database. What we propose is strictly a mathematical comparison that does not account for biological or health endpoints, chemical structure activity, or other parameters of AEGL derivations (e.g., species, uncertainty factors, time-scaling extrapolations). Yet, not accounting for these specific factors in the present analysis enabled us to assess the overall landscape of the AEGL database and find a dependence of the model on exposure duration and severity threshold. We may not have observed or been able to interpret this trend if too many variables were in the initial model. In future analysis, a multivariate model will be considered to evaluate the significance of these factors and their potential interactions in the model and on quality of AEGL estimates (Woodall, 2005).

In conclusion, the statistical DLR models presented in the study lay the groundwork for further investigation of its utility to estimate provisional AEGLs for existing and new compounds without HGV values assigned. The applicability of such methods is especially important when empirical data and benchmark dose concentrations are insufficient. The statistical DLR models can also be used for quality control of the previous AEGL development process in comparison to current changes in the AEGL program. I*n silico* methods, like the one proposed in the present study, are not intended to replace biological and toxicological evidence. Instead, they offer a complementary approach when such evidence is unavailable, budget is limited, and/or rapid assessment is necessary, i.e. an emergency response to an airborne chemical release.

V. CONCLUSIONS

The present research proposes an *in silico* statistical approach for rapid estimation of inhalation provisional health guidance values (pHGV) on the AEGL-1, -2, -3 compatibility scale for compounds with unassigned HGVs. This information would complement existing occupational and emergency comparison values by providing estimates of acute exposure durations (10 min to 8 h) at multiple health toxicity endpoints (Appendix 11). The method applied Pearson correlation and Deming linear regression analyses to the overall AEGL database to assess the trends in concentrations by exposure durations and severity thresholds. Our findings suggested that the proposed DLR models were statistically valid and predictive of unassigned AEGL values for compounds in the database. A novel construction of the bootstrap prediction intervals enabled sensitivity analyses of the models to estimate future AEGL estimates at the 95% probability (e.g., within 95% reference limits). Model performance was dependent on the severity threshold and exposure duration of the cross-extrapolated quantities. External validation using occupational exposure limits showed that cross-extrapolation estimates were sound. The research contributes to public health by proposing a time and cost-efficient statistical approach for AEGL derivation that can be used during emergency response to chemical releases in which no chemical information is available. With the national emphasis on *in silico* risk assessment methods in light of funding shortages, the proposed statistical method provides the foundation for further work in the field.

VI. RECOMMENDATIONS/FUTURE RESEARCH

Our understanding of cross-threshold extrapolation within and across HGV databases is still emerging since the involved health endpoints and exposure durations vary on case-by-case basis. Nevertheless, with the lack of short-term exposure HGVs and funding cutbacks in the AEGL Program, the need for surrogate risk assessment methods is ever-growing. Recommendations for future research would be to evaluate the role of structure-activity relationships, time-scaling, uncertainty factors, and mechanisms of toxicity in the model in influencing AEGLs predictions. These further analyses may explain the observed high correlations and linearity across exposure durations and severity thresholds established in the present study on the $\log_{10}$-scale. These relationships can then be analyzed using Quantitative Structure-Activity Relationship (QSAR) modeling, which provides insights into important molecular features and properties associated with the toxicity of compounds. Yet, a case-by-case approach should also be taken to evaluate the validity of AEGLs predictions for each compound. AEGL estimates from the DLR statistical model should be compared with empirical data and if available, benchmark concentration values, to ensure scientific credibility and data consistency. In addition, external comparisons with other acute reference values not discussed in the current study should also be considered, such as California EPA's reference exposure limits (REL) (OEHHA 2012) and the ATSDR's Minimal Risk Levels (MRLs) (ATSDR 2012) (Appendix 13).

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VII. TABLES /FIGURES

i. Tables:

Table 1. Database of the 273 inhalable compounds in which AEGL values were developed. For each compound, information of its published units, CAS registry number, molecular weight (MW), stage of the AEGL development process, and $\log_{10}$AEGL values in parts per million (ppm) were included. Unassigned AEGL values were shown as "NR" for not recommended.

Table 2. Descriptive statistics and tests of normality for AEGLs at each exposure duration and severity health threshold. A high frequency of unassigned values existed in the AEGL-1 threshold (105 -109 compounds). Measures of central tendency include the mean, standard deviation, and the maximum and minimum for each AEGL level. Measures of normality, variance, and skewness indicated that the AEGL data was heavily right skewed. The AEGL data was normalized after $\log_{10}$ transformation.

Table 3. A fifteen-by-fifteen Pearson correlation matrix of AEGLs across all five exposure duration (1/6 to 8 h) and three health severity thresholds (-1, -2, -3). Each cell represented the correlation of two duration-and-threshold-specific AEGL levels. All correlation coefficients (*r*) were at least 0.88. The highest correlations were observed for within threshold AEGL pairs (dark green cells). The lowest correlations were observed for all cross-threshold AEGL pairs at the 10 min. exposure durations (light green cells).

Table 4. Deming linear regression estimates for each of the 105 unique duration-and-threshold specific AEGL pairs. Estimates include the slope (B1), intercept (Bo), and their standard errors (SE) and 95% confidence intervals (CIs). Hypothesis testing of database comparability showed statistical identity of Deming slopes and y-intercepts (Reject Ho?: N=no, Y=yes). Cells highlighted with purple font have statistically identical slopes (95% CI_{B1} includes 1), and cells highlighted with green font have statistically identical intercepts (95% CI_{Bo} includes 0).

Table 5. Distribution of duration-and-threshold-specific AEGL pairs with observed statistical identity. Cells highlighted in purple indicate AEGL pairs with statistically identical slopes and cells with 'a_o' indicate AEGL pairs with statistically identical intercepts.

Table 6. Distribution of identical surrogate values across AEGL levels of varying exposure durations and health severity thresholds. The numbers represent the frequency of compounds with identical AEGL values in their corresponding duration-and-threshold-specific AEGL level. Darker purple cells also indicate AEGL levels with a higher frequency of identical surrogates. The AEGL-1 threshold had the most compounds in which identical values were used across multiple exposure durations.

Table 7. Test of DLR model performance. AEGL pair models ranked by their Pearson correlations (high, middle, and low) were assessed for the percentage of compounds with AEGLs estimates falling within a magnitude of 3, 10, 100, and >100-folds difference from actual AEGL values. Models with high Pearson correlation coefficients had more compounds with AEGL estimates within a 3-fold difference than for models with the middle and lowest Pearson correlations. Yet, AEGL models with the narrowest 95% PIs, regardless of correlation magnitude, had highest percentage of compounds with estimates within a 3-fold difference.

Table 8. Selection criteria for the "best" predictive models. AEGL model pairs with the best model performance for each duration-and-threshold-specific AEGL level were ranked by (1) the magnitude difference of their AEGL estimates to actual values, (2) width of their 95% PIs, (3) residual plots, and (4) their Pearson correlation coefficient magnitude. Alternative model pairs, within and cross-threshold, were presented in cases where an AEGL predictive value for the best model is unassigned for a compound.
Table 9. Compounds in the AEGL database with NIOSH and ACGIH's occupational exposure limits (OEL) assigned. Compounds highlighted in red have unassigned AEGL-1 values (NA = not available).

Table 10. Deming linear regression assessment of data comparability within OELs, and between OELs and assigned AEGL values. Comparisons of OELs with each other showed statistical identity of slopes (95% CI contain 1) for all OEL pairs. Comparisons of OEL-STELs with AEGLs showed all pairs had statistically identical slopes, and that the highest correlated pairs were between OEL-STELs and AEGL-1s and -2s at the 4 h and 8 h, and AEGL-2 at 1 h. Comparisons between OEL-TWAs and AEGLs showed statistical identity for all pairs except for ACGIH TLV-TWAs and AEGL-2s at the 4 and 8h. The highest correlation also existed between OEL-TWA pairs with AEGL-1s and -2s at the 4 h and 8 h. The statistical identity in slopes of OELs especially with AEGL-1s at the 4 h and 8 h exposure durations (highlighted in red) indicate that their data are comparable. Hence, OEL values can then be used as a crude external validation for DLR derived AEGL-1 estimates at 4h and 8h for compounds with unassigned values.

Table 11. Internal and external cross-validation of AEGL estimates from the proposed "best" DLR models. For the 14 compounds with unassigned AEGL-1 values, AEGL-1 and -2 estimates at the 4 h and 8 h exposure duration were derived from the best DLR model pairs. These estimates were compared to OEL and known AEGL-2 values to assess validity of model estimates for the respective compounds. For each of the 4 DLR models employed, X = AEGL predictor value for DLR model and Y=AEGL-1 or -2 at the 4 h or 8 h duration. AEGL-1 estimates were assumed to be statistically valid if their 95% PIs included the OEL value for each compound (highlighted blue or green cells). At the 95% prediction level, 8/14 compounds had statistically similar estimates between AEGL-1 and OEL-TWA values and 3/14 compounds had statistically similar estimates between AEGL-1 and OEL-STEL values.

ii. Figures

Figure 1. Frequency of unassigned AEGLs in the database. 115 (42%) compounds had at least two unassigned AEGL values. From these, 109 (91%) were concentrated in the AEGL-1 threshold. Only 6 compounds had unassigned values in the AEGL-2 threshold and 10 had unassigned values in the AEGL-3 threshold.

Figure 2. For each of the 15 duration-and-threshold-specific AEGL levels (y-axis), 14 cross-threshold and/or cross-exposure-duration univariate DLR models were constructed. Their respective slope (red), 95% CIs (blue) and 95% PIs (green) of the regression line, and correlation coefficients are presented. The highest correlations for cross-threshold models are in red. Assessment of the 95% PI width and correlation coefficient for all models showed similar trends: DLR models with narrower 95% PIs generally had higher correlations.

Figure 3. Residual plots of AEGL estimates for the 15 duration-and-threshold-specific AEGL levels. Three AEGL pair models were selected for each, ranked by the magnitude of their correlation coefficients: highest (blue), middle (orange), and lowest (yellow). Normality and proximity of predictions to actual values were assessed by the scatter and distance of the AEGL estimates about the horizontal axis. Horizontal green lines indicate the cut-off levels for the magnitude difference between predicted and actual values: 3, 10, and 100-fold difference.

Figure 4. Line graphs of DLR model performance for each AEGL pair models ranked by their Pearson correlations (highest, middle, and lowest). The percentage of compounds with AEGLs estimates falling within a magnitude of 3 (blue), 10 (red), and 100-folds (green) difference from actual AEGLs were assessed. Models with higher Pearson correlation coefficients mostly had more compounds with AEGL estimates within a 3-fold difference. Yet, for 6 models with lower correlations but narrower 95% PI widths (highlighted yellow), the percentage of compounds with AEGL estimates within a 3-fold difference was the highest out of all model types. Although a relationship between Pearson correlations and 95% PI width seems to exist, model performance was observed to be more dependent on 95% PI width.

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
1	1,1,1-Trichloroethane	ppm	71-55-6	133.4	I	2.30E+02	2.30E+02	2.30E+02	2.30E+02	2.30E+02	9.30E+02	6.70E+02	6.00E+02	3.80E+02	3.10E+02	4.20E+03	4.20E+03	4.20E+03	2.70E+03	2.10E+03
2	1,1-Dimethylhydrazine	ppm	57-14-7	60.1	F	NR	NR	NR	NR	NR	1.80E+01	6.00E+00	3.00E+00	7.50E-01	3.80E-01	6.50E+01	2.20E+01	1.10E+01	2.70E+00	1.40E+00
3	1,2,3-Trimethylbenzene	ppm	526-73-8	120.2	I	1.80E+02	1.80E+02	1.40E+02	9.00E+01	4.50E+01	4.60E+02	4.60E+02	3.60E+02	2.30E+02	1.50E+02	NR	NR	NR	NR	NR
4	1,2,4-Trimethylbenzene	ppm	95-63-6	120.2	I	1.80E+02	1.80E+02	1.40E+02	9.00E+01	4.50E+01	4.60E+02	4.60E+02	3.60E+02	2.30E+02	1.50E+02	NR	NR	NR	NR	NR
5	1,2-butyleneoxide	ppm	106-88-7	72.1	I	7.20E+01	7.20E+01	7.20E+01	7.20E+01	7.20E+01	1.40E+02	1.40E+02	1.40E+02	1.40E+02	1.40E+02	4.10E+02	4.10E+02	3.30E+02	2.10E+02	2.10E+02
6	1,2-Dimethylhydrazine	ppm	540-73-8	60.1	F	NR	NR	NR	NR	NR	1.80E+01	6.00E+00	3.00E+00	7.50E-01	3.80E-01	6.50E+01	2.20E+01	1.10E+01	2.70E+00	1.40E+00
7	1,3,5-Trimethylbenzene	ppm	108-67-8	120.2	I	1.80E+02	1.80E+02	1.40E+02	9.00E+01	4.50E+01	4.60E+02	4.60E+02	3.60E+02	2.30E+02	1.50E+02	NR	NR	NR	NR	NR
8	1,3-Butadiene	ppm	106-99-0	54.1	I	6.70E+02	6.70E+02	6.70E+02	6.70E+02	6.70E+02	6.70E+03	6.70E+03	5.30E+03	3.40E+03	2.70E+03	2.70E+04	2.70E+04	2.20E+04	1.40E+04	6.80E+03
9	1,4-Dioxane	ppm	123-91-1	88.1	I	1.70E+01	1.70E+01	1.70E+01	1.70E+01	1.70E+01	5.80E+02	4.00E+02	3.20E+02	2.00E+02	1.00E+02	9.50E+02	9.50E+02	7.60E+02	4.80E+02	2.40E+02
10	2,4-TolueneDiisocyanate	ppm	584-84-9	174.2	F	2.00E-02	2.00E-02	2.00E-02	1.00E-02	1.00E-02	2.40E-01	1.70E-01	8.30E-02	2.10E-02	2.10E-02	6.50E-01	6.50E-01	5.10E-01	3.20E-01	1.60E-01
11	2,6-Toluenediisocyanate	ppm	91-08-7	174.2	F	2.00E-02	2.00E-02	2.00E-02	1.00E-02	1.00E-02	2.40E-01	1.70E-01	8.30E-02	2.10E-02	2.10E-02	6.50E-01	6.50E-01	5.10E-01	3.20E-01	1.60E-01
12	2-Ethylhexyl-chloroformate	ppm	24468-13-1	192.7	I	NR	NR	NR	NR	NR	1.20E+00	1.20E+00	9.70E-01	6.00E-01	3.00E-01	3.60E+00	3.60E+00	2.90E+00	1.80E+00	9.10E-01
13	Acetaldehyde	ppm	75-07-0	44.1	I	4.50E+01	4.50E+01	4.50E+01	4.50E+01	4.50E+01	3.40E+02	3.40E+02	2.70E+02	1.70E+02	1.10E+02	1.10E+03	1.10E+03	8.40E+02	5.30E+02	2.60E+02
14	Acetone	ppm	67-64-1	58.1	I	2.00E+02	2.00E+02	2.00E+02	2.00E+02	2.00E+02	9.30E+03	4.90E+03	3.20E+03	1.40E+03	9.50E+02	1.60E+04	8.60E+03	5.70E+03	2.50E+03	1.70E+03
15	Acetonecyanohydrin	ppm	75-86-5	85.1	F	2.50E+00	2.50E+00	2.00E+00	1.30E+00	1.00E+00	1.70E+01	1.00E+01	7.10E+00	3.50E+00	2.50E+00	2.70E+01	2.10E+01	1.50E+01	8.60E+00	6.60E+00
16	Acetonitrile	ppm	75-05-8	41.1	I	1.30E+01	1.30E+01	1.30E+01	1.30E+01	1.30E+01	4.90E+02	4.90E+02	3.20E+02	1.30E+02	8.60E+01	1.00E+03	1.00E+03	6.70E+02	2.80E+02	1.80E+02
17	Acrolein	ppm	107-02-8	56.1	F	3.00E-02	3.00E-02	3.00E-02	3.00E-02	3.00E-02	4.40E-01	1.80E-01	1.00E-01	1.00E-01	1.00E-01	6.20E+00	2.50E+00	1.40E+00	4.80E-01	2.70E-01
18	Acrylicacid	ppm	79-10-7	72.1	I	1.50E+00	1.50E+00	1.50E+00	1.50E+00	1.50E+00	6.80E+01	6.80E+01	4.60E+01	2.10E+01	1.40E+01	4.80E+02	2.60E+02	1.80E+02	8.50E+01	5.80E+01
19	Acrylonitrile	ppm	107-13-1	53.1	I	4.60E+00	4.60E+00	4.60E+00	4.60E+00	4.60E+00	2.90E+02	1.10E+02	5.70E+01	1.60E+01	8.60E+00	4.80E+02	1.80E+02	1.00E+02	3.50E+01	1.90E+01
20	Adamsite	mg/m^3	578-94-9	277.6	I	1.76E-02	3.61E-03	1.41E-03	1.94E-04	7.32E-05	8.55E-01	5.99E-01	2.29E-01	3.17E-02	1.23E-02	1.85E+00	1.50E+00	5.64E-01	8.02E-02	3.00E-02
21	AgentGB(Sarin)	ppm	107-44-8	140.1	F	1.20E-03	6.80E-04	4.80E-04	2.40E-04	1.70E-04	1.50E-02	8.50E-03	6.00E-03	2.90E-03	2.20E-03	6.40E-02	3.20E-02	2.20E-02	1.20E-02	8.70E-03
22	AgentGD(Soman)	ppm	96-64-0	182.2	F	4.60E-04	2.60E-04	1.80E-04	9.10E-05	6.50E-05	5.70E-03	3.30E-03	2.20E-03	1.20E-03	8.50E-04	4.90E-02	2.50E-02	1.70E-02	9.10E-03	6.60E-03
23	AgentGF	ppm	329-99-7	180.2	F	4.90E-04	2.80E-04	2.00E-04	1.00E-04	7.00E-05	6.20E-03	3.50E-03	2.40E-03	1.30E-03	9.10E-04	5.30E-02	2.70E-02	1.80E-02	9.80E-03	7.10E-03
24	AgentVX	ppm	50782-69-9	267.4	F	5.20E-05	3.00E-05	1.60E-05	9.10E-06	6.50E-06	6.50E-04	3.80E-04	2.70E-04	1.40E-04	9.50E-05	2.70E-03	1.40E-03	9.10E-04	4.80E-04	3.50E-04
25	Aldicarb	mg/m^3	116-06-3	190.3	P	NR	NR	NR	NR	NR	2.06E-02	1.41E-02	1.12E-02	6.81E-03	3.47E-03	6.04E-02	4.11E-02	3.34E-02	2.06E-02	1.04E-02
26	Allylalcohol	ppm	107-18-6	58.1	I	9.30E+00	6.40E+00	5.10E+00	2.20E+00	1.00E+00	8.70E+01	2.70E+01	1.30E+01	3.10E+00	1.50E+00	2.60E+02	8.20E+01	4.00E+01	9.30E+00	4.50E+00
27	AllylAmine	ppm	107-11-9	57.1	F	4.20E-01	4.20E-01	4.20E-01	4.20E-01	4.20E-01	3.30E+00	3.30E+00	3.30E+00	1.80E+00	1.20E+00	1.50E+02	4.00E+01	1.80E+01	3.50E+00	2.30E+00
28	Allylchloride	ppm	107-05-1	76.5	I	2.80E+00	2.80E+00	2.80E+00	2.80E+00	2.80E+00	6.90E+01	6.90E+01	5.40E+01	3.40E+01	2.20E+01	1.80E+02	1.80E+02	1.40E+02	9.00E+01	6.00E+01
29	Allylchloroformate	ppm	2937-50-0	120.5	I	NR	NR	NR	NR	NR	1.30E+00	8.70E-01	7.00E-01	1.80E-01	9.00E-02	3.80E+00	2.60E+00	2.10E+00	5.30E-01	2.60E-01
30	Allyltrichlorosilane	ppm	107-37-9	175.5	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
31	Aluminum phosphide	ppm	20859-73-8	58.0	F	NR	NR	NR	NR	NR	4.00E+00	4.00E+00	2.00E+00	5.00E-01	2.50E-01	7.20E+00	7.20E+00	3.60E+00	9.00E-01	4.50E-01
32	Ammonia	ppm	7664-41-7	17.0	F	3.00E+01	3.00E+01	3.00E+01	3.00E+01	3.00E+01	2.20E+02	2.20E+02	1.60E+02	1.10E+02	1.10E+02	2.70E+03	1.60E+03	1.10E+03	5.50E+02	3.90E+02
33	Amyltrichlorosilane	ppm	107-72-2	205.6	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
34	Aniline	ppm	62-53-3	93.1	F	4.80E+01	1.60E+01	8.00E+00	2.00E+00	1.00E+00	7.20E+01	2.40E+01	1.20E+01	3.00E+00	1.50E+00	1.20E+02	4.00E+01	2.00E+01	5.00E+00	2.50E+00
35	Arsenic trioxide	mg/m^3	1327-53-3	197.8	I	NR	NR	NR	NR	NR	4.58E-01	4.58E-01	3.71E-01	2.35E-01	1.48E-01	1.36E+00	1.36E+00	1.13E+00	7.05E-01	4.58E-01

Table 1. Database of the 273 inhalable compounds in which AEGL values were developed. For each compound, information of its published units, CAS registry number, molecular weight (MW), stage of the AEGL development process, and $\log_{10}$AEGL values in parts per million (ppm) were included. Unassigned AEGL values were shown as "NR" for not recommended.

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
36	Arsine	ppm	7784-42-1	74.9	F	NR	NR	NR	NR	NR	3.00E-01	2.10E-01	1.70E-01	4.00E-02	2.00E-02	9.10E-01	6.30E-01	5.00E-01	1.30E-01	6.00E-02
37	Automotive Gasoline (unleaded)	mg/m^3	NA	NA	P	2.44E+02	2.44E+02	2.44E+02	2.44E+02	2.44E+02	2.51E+03	2.51E+03	2.51E+03	2.51E+03	2.51E+03	NR	NR	NR	NR	NR
38	Benzene	ppm	71-43-2	78.1	I	1.30E+02	7.30E+01	5.20E+01	1.80E+01	9.00E+00	2.00E+03	1.10E+03	8.00E+02	4.00E+02	2.00E+02	9.70E+03	5.60E+03	4.00E+03	2.00E+03	9.90E+02
39	Benzonitrile	ppm	100-47-0	103.1	I	NR	NR	NR	NR	NR	3.90E+01	2.70E+01	2.20E+01	1.10E+01	5.60E+00	1.00E+02	7.10E+01	5.60E+01	2.30E+01	1.10E+01
40	Benzylchloroformate	ppm	501-53-1	170.6	I	NR	NR	NR	NR	NR	1.20E+00	1.20E+00	9.70E-01	6.30E-01	3.10E-01	3.70E+00	3.70E+00	2.90E+00	1.90E+00	9.30E-01
41	Biphenyl	ppm	92-52-4	154.2	I	NR	NR	NR	NR	NR	1.20E+01	1.20E+01	9.60E+00	6.00E+00	4.40E+00	NR	NR	NR	NR	NR
42	Bis (chloromethyl) ether	ppm	542-88-1	115.0	I	NR	NR	NR	NR	NR	5.50E-02	5.50E-02	4.40E-02	2.80E-02	2.00E-02	2.30E-01	2.30E-01	1.80E-01	1.10E-01	7.50E-02
43	Boron trifluoride	mg/m^3	7637-07-2	67.8	I	9.02E-01	9.02E-01	9.02E-01	9.02E-01	9.02E-01	1.70E+01	1.70E+01	1.33E+01	8.66E+00	4.33E+00	5.05E+01	5.05E+01	3.97E+01	2.60E+01	1.30E+01
44	Borontribromide	ppm	10294-33-4	250.5	I	3.30E-01	3.30E-01	3.30E-01	3.30E-01	3.30E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.50E+02	8.30E+01	4.00E+01	1.00E+01	1.00E+01
45	Bromine	ppm	7726-95-6	79.9	F	3.30E-02	3.30E-02	3.30E-02	3.30E-02	3.30E-02	5.50E-01	3.30E-01	2.40E-01	1.30E-01	9.50E-02	1.90E+01	1.20E+01	8.50E+00	4.50E+00	3.30E+00
46	Brominechloride	ppm	13863-41-7	115.4	I	5.00E-01	5.00E-01	5.00E-01	5.00E-01	5.00E-01	3.20E+00	3.20E+00	2.50E+00	1.60E+00	1.20E+00	9.50E+00	9.50E+00	7.60E+00	4.80E+00	3.50E+00
47	Brominepentafluoride	ppm	7789-30-2	174.9	I	NR	NR	NR	NR	NR	3.00E+00	2.00E+00	1.00E+00	4.80E-01	3.30E-01	7.90E+01	5.50E+01	3.30E+01	8.30E+00	4.20E+00
48	Brominetrifluoride	ppm	7787-71-5	136.9	I	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	8.10E+00	3.50E+00	2.00E+00	7.00E-01	4.10E-01	8.40E+01	3.60E+01	2.10E+01	7.30E+00	7.30E+00
49	Bromoacetone	ppm	598-31-2	137.0	I	1.10E-02	1.10E-02	1.10E-02	1.10E-02	1.10E-02	1.40E+00	5.70E-01	3.30E-01	1.10E-01	6.30E-02	4.10E+00	1.70E+00	9.80E-01	3.20E-01	1.90E-01
50	Butane	ppm	106-97-8	58.1	I	1.00E+04	6.90E+03	5.50E+03	5.50E+03	5.50E+03	2.40E+04	1.70E+04	1.70E+04	1.70E+04	1.70E+04	7.70E+04	5.30E+04	5.30E+04	5.30E+04	5.30E+04
51	Butyltrichlorosilane	ppm	7521-80-4	191.6	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
52	BZ	mg/m^3	6/2/6581	337.4	I	NR	NR	NR	NR	NR	1.59E-02	5.36E-03	2.68E-03	NR	NR	2.97E-01	1.01E-01	5.00E-02	NR	NR
53	Cadmium	mg/m^3	7440-43-9	112.4	I	2.83E-02	2.83E-02	2.17E-02	1.37E-02	8.91E-03	3.04E-01	2.09E-01	1.65E-01	8.70E-02	4.35E-02	1.85E+00	1.28E+00	1.02E+00	4.13E-01	2.02E-01
54	Calcium cyanide	mg/m^3	592-01-8	92.1	I	1.24E+00	1.24E+00	1.00E+00	6.32E-01	5.00E-01	8.42E+00	5.00E+00	3.42E+00	1.74E+00	1.24E+00	1.34E+01	1.03E+01	7.37E+00	4.21E+00	3.16E+00
55	Calcium phosphide	ppm	1305-99-3	182.2	F	NR	NR	NR	NR	NR	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	3.60E+00	3.60E+00	1.80E+00	4.50E-01	2.30E-01
56	Carbon monoxide	ppm	630-08-0	28.0	F	NR	NR	NR	NR	NR	4.20E+02	1.50E+02	8.30E+01	3.30E+01	2.70E+01	1.70E+03	6.00E+02	3.30E+02	1.50E+02	1.30E+02
57	Carbondisulfide	ppm	75-15-0	76.1	F	1.70E+01	1.70E+01	1.30E+01	8.40E+00	6.70E+00	2.00E+02	2.00E+02	1.60E+02	1.00E+02	5.00E+01	6.00E+02	6.00E+02	4.80E+02	3.00E+02	1.50E+02
58	Carbontetrachloride	ppm	56-23-5	153.8	I	5.80E+01	5.80E+01	4.40E+01	2.50E+01	1.90E+01	3.80E+02	2.50E+02	1.90E+02	1.00E+02	8.10E+01	1.10E+03	6.80E+02	5.20E+02	3.00E+02	2.20E+02
59	Carbonylfluoride	ppm	353-50-4	66.0	I	NR	NR	NR	NR	NR	3.50E-01	3.50E-01	2.80E-01	1.70E-01	8.70E-02	1.00E+00	1.00E+00	8.30E-01	5.20E-01	2.60E-01
60	CarbonylSulfide	ppm	463-58-1	60.1	I	NR	NR	NR	NR	NR	6.90E+01	6.90E+01	5.50E+01	3.40E+01	2.30E+01	1.90E+02	1.90E+02	1.50E+02	9.50E+01	4.80E+01
61	Chlorine	ppm	7782-50-5	70.9	F	5.00E-01	5.00E-01	5.00E-01	5.00E-01	5.00E-01	2.80E+00	2.80E+00	2.00E+00	1.00E+00	7.10E-01	5.00E+01	2.80E+01	2.00E+01	1.00E+01	7.10E+00
62	Chlorine pentafluoride	ppm	13637-63-3	130.4	I	3.00E-01	3.00E-01	3.00E-01	NR	NR	3.00E+00	2.00E+00	1.00E+00	4.80E-01	3.30E-01	2.10E+01	1.20E+01	8.00E+00	3.90E+00	2.70E+00
63	Chlorinedioxide	ppm	10049-04-4	67.5	F	1.50E-01	1.50E-01	1.50E-01	1.50E-01	1.50E-01	1.40E+00	1.40E+00	1.10E+00	6.90E-01	4.50E-01	3.00E+00	3.00E+00	2.40E+00	1.50E+00	9.80E-01
64	Chlorinetrifluoride	ppm	7790-91-2	92.4	F	1.20E-01	1.20E-01	1.20E-01	1.20E-01	1.20E-01	8.10E+00	3.50E+00	2.00E+00	7.00E-01	4.10E-01	8.40E+01	3.60E+01	2.10E+01	7.30E+00	7.30E+00
65	Chloroacetaldehyde	ppm	107-20-0	78.5	I	2.30E+00	2.30E+00	1.30E+00	4.00E-01	2.20E-01	9.80E+00	3.90E+00	2.20E+00	6.90E-01	3.90E-01	4.40E+01	1.80E+01	9.90E+00	3.10E+00	1.80E+00
66	Chloroacetone	ppm	78-95-5	92.5	I	NR	NR	NR	NR	NR	8.00E+00	5.50E+00	4.40E+00	1.10E+00	5.30E-01	2.40E+01	1.70E+01	1.30E+01	3.30E+00	1.60E+00
67	Chloroacetonitrile	ppm	107-14-2	75.5	I	NR	NR	NR	NR	NR	4.90E+01	4.90E+01	3.20E+01	1.30E+01	8.60E+00	1.00E+02	1.00E+02	6.70E+01	2.80E+01	1.80E+01
68	Chloroacetylchloride	ppm	79-04-9	112.9	I	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	2.90E+00	2.00E+00	1.60E+00	4.00E-01	2.00E-01	9.50E+01	6.60E+01	5.20E+01	1.30E+01	6.50E+00
69	Chlorobenzene	ppm	108-90-7	112.6	I	1.00E+01	1.00E+01	1.00E+01	1.00E+01	1.00E+01	4.30E+02	3.00E+02	1.50E+02	1.50E+02	1.50E+02	1.10E+03	8.00E+02	4.00E+02	4.00E+02	4.00E+02
70	Chloroform	ppm	67-66-3	119.4	I	NR	NR	NR	NR	NR	1.20E+02	8.00E+01	6.40E+01	4.00E+01	2.90E+01	4.00E+03	4.00E+03	3.20E+03	2.00E+03	1.60E+03

Table 1 (2 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
71	Chloromethylmethylether	ppm	107-30-2	80.5	I	NR	NR	NR	NR	NR	6.00E-01	6.00E-01	4.70E-01	3.00E-01	2.20E-01	2.60E+00	2.60E+00	2.00E+00	1.30E+00	9.30E-01
72	Chloromethyltrichlorosilane	ppm	1558-25-4	183.9	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
73	Chloropicrin	ppm	76-06-2	164.4	I	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	1.50E-01	1.50E-01	1.50E-01	1.50E-01	1.50E-01	2.00E+00	2.00E+00	1.40E+00	7.90E-01	5.80E-01
74	Chlorosulfonic acid	mg/m^3	7790-94-5	116.5	I	2.10E-02	2.10E-02	2.10E-02	2.10E-02	2.10E-02	9.22E-01	9.22E-01	9.22E-01	9.22E-01	9.22E-01	9.43E+00	6.50E+00	5.24E+00	1.28E+00	1.28E+00
75	cis-1,2-Dichloroethylene	ppm	156-59-2	96.9	F	1.40E+02	1.40E+02	1.40E+02	1.40E+02	1.40E+02	5.00E+02	5.00E+02	5.00E+02	3.40E+02	2.30E+02	8.50E+02	8.50E+02	8.50E+02	6.20E+02	3.10E+02
76	cis-Crotonaldehyde	ppm	4170-30-3	70.1	F	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	2.70E+01	8.90E+00	4.40E+00	1.10E+00	5.60E-01	4.40E+01	2.70E+01	1.40E+01	2.60E+00	1.50E+00
77	Cumene	ppm	98-82-8	120.2	I	5.00E+01	5.00E+01	5.00E+01	5.00E+01	5.00E+01	5.50E+02	3.80E+02	3.00E+02	1.90E+02	1.30E+02	1.30E+03	9.20E+02	7.30E+02	4.60E+02	3.00E+02
78	Cyanogen	ppm	460-19-5	60.1	I	2.50E+00	2.50E+00	2.00E+00	1.30E+00	1.00E+00	5.00E+01	1.70E+01	8.30E+00	4.30E+00	4.30E+00	1.50E+02	5.00E+01	2.50E+01	1.30E+01	1.30E+01
79	Cyclohexylamine	ppm	108-91-8	99.2	F	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.10E+01	1.10E+01	8.60E+00	5.40E+00	2.70E+00	3.80E+01	3.80E+01	3.00E+01	1.90E+01	9.50E+00
80	Cyclohexylisocyanate	ppm	3173-53-3	125.2	I	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	1.30E-01	1.30E-01	1.00E-01	6.40E-02	4.20E-02
81	Diborane	ppm	19287-45-7	25.7	F	NR	NR	NR	NR	NR	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	7.30E+00	7.30E+00	3.70E+00	9.20E-01	4.60E-01
82	Dibromoethane	ppm	106-93-4	187.9	I	5.20E+01	2.60E+01	1.70E+01	7.10E+00	4.60E+00	7.30E+01	3.70E+01	2.40E+01	1.00E+01	6.50E+00	1.70E+02	7.60E+01	4.60E+01	1.70E+01	1.00E+01
83	Dichloroacetylchloride	ppm	79-36-7	147.4	I	4.00E-02	4.00E-02	4.00E-02	4.00E-02	4.00E-02	2.90E+00	2.00E+00	1.60E+00	4.00E-01	2.00E-01	9.50E+01	6.60E+01	5.20E+01	1.30E+01	6.50E+00
84	Dichlorodimethylsilane	ppm	75-78-5	129.1	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
85	Dichlorophenyltrichlorosilane	ppm	27137-85-5	280.4	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
86	Dichlorosilane	ppm	4109-96-0	101.0	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
87	Dichlorvos	ppm	62-73-7	221.0	P	1.10E-01	1.10E-01	1.10E-01	1.10E-01	1.10E-01	5.60E-01	5.60E-01	5.60E-01	5.60E-01	5.60E-01	8.00E+00	8.00E+00	8.00E+00	8.00E+00	8.00E+00
88	Dicrotophos	mg/m^3	141-66-2	237.2	P	NR	NR	NR	NR	NR	5.48E-02	3.82E-02	3.00E-02	7.54E-03	3.82E-03	1.65E-01	1.14E-01	9.09E-02	2.27E-02	1.14E-02
89	Diethyldichlorosilane	ppm	1719-53-5	157.1	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
90	Diketene	ppm	674-82-8	84.1	I	NR	NR	NR	NR	NR	1.10E+01	7.70E+00	6.00E+00	1.50E+00	7.70E-01	3.30E+01	2.30E+01	1.80E+01	4.50E+00	2.30E+00
91	Dimethyl phosphite	ppm	868-85-9	109.0	I	NR	NR	NR	NR	NR	1.20E+02	1.20E+02	9.50E+01	6.00E+01	3.90E+01	1.90E+02	1.90E+02	1.50E+02	9.60E+01	6.30E+01
92	Dimethylamine	ppm	124-40-3	45.1	I	1.00E+01	1.00E+01	1.00E+01	1.00E+01	1.00E+01	1.30E+02	8.50E+01	6.60E+01	4.00E+01	3.20E+01	4.80E+02	3.20E+02	2.50E+02	1.50E+02	1.20E+02
93	Dimethylchlorosilane	ppm	1066-35-9	93.6	I	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.00E+02	4.30E+01	2.20E+01	1.10E+01	1.10E+01	6.20E+02	2.10E+02	1.00E+02	2.60E+01	2.60E+01
94	Dimethylsulfate	ppm	77-78-1	126.1	I	3.50E-02	3.50E-02	2.40E-02	1.20E-02	8.70E-03	1.70E-01	1.70E-01	1.20E-01	6.10E-02	4.30E-02	4.00E+00	2.30E+00	1.60E+00	8.20E-01	5.80E-01
95	Diphenylchloroarsine	mg/m^3	712-48-1	264.6	I	NR	NR	NR	NR	NR	1.02E-01	7.31E-02	3.61E-02	9.06E-03	4.53E-03	3.14E-01	2.22E-01	1.11E-01	2.77E-02	1.39E-02
96	Diphenyldichlorosilane	ppm	80-10-4	253.2	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
97	Disulfurdichloride	ppm	10025-67-9	135.0	I	6.70E-01	6.70E-01	5.30E-01	3.30E-01	1.70E-01	8.10E+00	8.10E+00	6.40E+00	4.00E+00	2.00E+00	1.90E+01	1.90E+01	1.50E+01	9.60E+00	4.80E+00
98	Dodecyltrichlorosilane	ppm	4484-72-4	303.8	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
99	Epichlorohydrin	ppm	106-89-8	92.5	I	5.70E+00	5.70E+00	5.70E+00	5.70E+00	5.70E+00	5.30E+01	5.30E+01	2.40E+01	1.40E+01	1.00E+01	5.70E+02	1.60E+02	7.20E+01	4.40E+01	3.00E+01
100	Ethyl chloroformate	ppm	541-41-3	108.5	I	NR	NR	NR	NR	NR	2.90E+00	2.00E+00	1.60E+00	4.00E-01	2.00E-01	8.80E+00	6.10E+00	4.80E+00	1.20E+00	6.00E-01

Table 1 (3 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
101	Ethylacrylate	ppm	140-88-5	100.1	I	8.30E+00	8.30E+00	8.30E+00	8.30E+00	8.30E+00	6.60E+01	4.50E+01	3.60E+01	1.90E+01	9.40E+00	9.50E+02	4.10E+02	2.40E+02	7.10E+01	4.10E+01
102	Ethylamine	ppm	75-04-7	45.1	I	7.50E+00	7.50E+00	7.50E+00	7.50E+00	7.50E+00	1.50E+02	7.60E+01	4.90E+01	2.20E+01	1.40E+01	8.10E+02	4.20E+02	2.70E+02	1.20E+02	7.60E+01
103	Ethylbenzene	ppm	100-41-4	106.2	I	3.30E+01	3.30E+01	3.30E+01	3.30E+01	3.30E+01	2.90E+03	1.60E+03	1.10E+03	6.60E+02	5.80E+02	4.70E+03	2.60E+03	1.80E+03	1.00E+03	9.10E+02
104	Ethylchlorothioformate	ppm	2941-64-2	124.6	I	NR	NR	NR	NR	NR	3.30E-01	3.30E-01	2.60E-01	1.70E-01	8.30E-02	1.00E+00	1.00E+00	7.90E-01	5.00E-01	2.50E-01
105	Ethyldichloroarsine	mg/m^3	598-14-1	174.9	I	NR	NR	NR	NR	NR	2.38E-02	7.97E-03	4.06E-03	NR	NR	7.27E-02	2.38E-02	1.20E-02	NR	NR
106	Ethylene diamine	ppm	107-15-3	60.1	F	NR	NR	NR	NR	NR	1.20E+01	1.20E+01	9.70E+00	6.10E+00	4.80E+00	2.50E+01	2.50E+01	2.00E+01	1.30E+01	1.00E+01
107	Ethylenechlorohydrin(2-Chloroethanol)	ppm	107-07-3	80.5	I	NR	NR	NR	NR	NR	7.00E+00	5.00E+00	4.00E+00	1.60E+00	7.70E-01	2.10E+01	1.50E+01	1.20E+01	4.70E+00	2.30E+00
108	Ethyleneimine	ppm	151-56-4	43.1	F	NR	NR	NR	NR	NR	3.30E+01	9.80E+00	4.60E+00	1.00E+00	4.70E-01	5.10E+01	1.90E+01	9.90E+00	2.80E+00	1.50E+00
109	Ethyleneoxide	ppm	75-21-8	44.1	F	NR	NR	NR	NR	NR	8.00E+01	8.00E+01	4.50E+01	1.40E+01	7.90E+00	3.60E+02	3.60E+02	2.00E+02	6.30E+01	3.50E+01
110	Ethylisocyanate	ppm	109-90-0	71.1	I	NR	NR	NR	NR	NR	7.00E-02	7.00E-02	5.30E-02	3.30E-02	2.30E-02	2.10E-01	2.10E-01	1.60E-01	1.00E-01	6.80E-02
111	Ethylmercaptan	ppm	75-08-1	62.1	I	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+02	1.50E+02	1.20E+02	7.70E+01	3.70E+01	4.50E+02	4.50E+02	3.60E+02	2.30E+02	1.10E+02
112	Ethyltrichlorosilane	ppm	115-21-9	163.5	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
113	Ethyphosphorodichloridate	ppm	1498-51-7	162.9	I	NR	NR	NR	NR	NR	1.10E+00	7.60E-01	6.00E-01	3.80E-01	1.90E-01	1.10E+01	7.60E+00	6.00E+00	3.80E+00	1.90E+00
114	Fenamiphos	mg/m^3	22224-92-6	303.4	P	NR	NR	NR	NR	NR	8.06E-02	6.45E-02	5.65E-02	4.27E-02	3.47E-02	2.42E-01	1.94E-01	1.69E-01	1.29E-01	1.05E-01
115	Fluorine	ppm	7782-41-4	38.0	F	1.70E+00	1.70E+00	1.70E+00	1.70E+00	1.70E+00	2.00E+01	1.10E+01	5.00E+00	2.30E+00	2.30E+00	3.60E+01	1.90E+01	1.30E+01	5.70E+00	5.70E+00
116	Formaldehyde	ppm	50-00-0	30.0	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	1.40E+01	1.40E+01	1.40E+01	1.40E+01	1.40E+01	1.00E+02	7.00E+01	5.60E+01	3.50E+01	3.50E+01
117	Furan	ppm	110-00-9	68.1	F	NR	NR	NR	NR	NR	1.20E+01	8.50E+00	6.80E+00	1.70E+00	8.50E-01	3.50E+01	2.40E+01	1.90E+01	4.80E+00	2.40E+00
118	Germane	ppm	7782-65-2	76.6	I	NR	NR	NR	NR	NR	3.00E-01	2.10E-01	1.70E-01	4.00E-02	2.00E-02	9.10E-01	6.30E-01	5.00E-01	1.30E-01	6.00E-02
119	HCFC141b	ppm	1717-00-6	117.0	F	1.00E+03	1.00E+03	1.00E+03	1.00E+03	1.00E+03	1.70E+03	1.70E+03	1.70E+03	1.70E+03	1.70E+03	3.00E+03	3.00E+03	3.00E+03	3.00E+03	3.00E+03
120	Hexafluoroacetone	ppm	684-16-2	166.0	I	NR	NR	NR	NR	NR	4.00E-01	4.00E-01	2.00E-01	5.00E-02	2.50E-02	1.60E+02	1.60E+02	8.00E+01	2.00E+01	1.00E+01
121	Hexafluoropropylene	ppm	116-15-4	150.0	I	1.50E+02	6.70E+01	4.00E+01	1.40E+01	8.30E+00	3.50E+02	1.50E+02	9.10E+01	3.20E+01	1.90E+01	1.80E+03	8.00E+02	4.80E+02	1.70E+02	1.00E+02
122	Hexane	ppm	110-54-3	86.2	I	NR	NR	NR	NR	NR	4.80E+03	3.30E+03	3.30E+03	3.30E+03	3.30E+03	1.20E+04	8.60E+04	8.60E+04	8.60E+04	8.60E+04
123	Hexyltrichlorosilane	ppm	928-65-4	219.6	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
124	HFC134A	ppm	811-97-2	102.0	F	8.00E+03	8.00E+03	8.00E+03	8.00E+03	8.00E+03	1.30E+04	1.30E+04	1.30E+04	1.30E+04	1.30E+04	2.70E+04	2.70E+04	2.70E+04	2.70E+04	2.70E+04
125	Hydrazine	ppm	302-01-2	32.0	F	1.00E-01	1.00E-01	1.00E-01	1.00E-01	1.00E-01	2.30E+01	1.60E+01	1.30E+01	3.10E+00	1.60E+00	6.40E+01	4.50E+01	3.50E+01	8.90E+00	4.40E+00
126	Hydrogen bromide	ppm	10035-10-6	80.9	I	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+02	5.00E+01	2.50E+01	1.30E+01	1.30E+01	7.40E+02	2.50E+02	1.20E+02	3.10E+01	3.10E+01
127	Hydrogenchloride	ppm	7647-01-0	36.5	F	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.00E+02	4.30E+01	2.20E+01	1.10E+01	1.10E+01	6.20E+02	2.10E+02	1.00E+02	2.60E+01	2.60E+01
128	Hydrogencyanide	ppm	74-90-8	27.0	F	2.50E+00	2.50E+00	2.00E+00	1.30E+00	1.00E+00	1.70E+01	1.00E+01	7.10E+00	3.50E+00	2.50E+00	2.70E+01	2.10E+01	1.50E+01	8.60E+00	6.60E+00
129	Hydrogenfluoride	ppm	7664-39-3	20.0	F	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	9.50E+01	3.40E+01	2.40E+01	1.20E+01	1.20E+01	1.70E+02	6.20E+01	4.40E+01	2.20E+01	2.20E+01
130	Hydrogeniodide	ppm	10034-85-2	127.9	I	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+02	5.00E+01	2.50E+01	1.30E+01	1.30E+01	7.40E+02	2.50E+02	1.20E+02	3.10E+01	3.10E+01
131	Hydrogenselenide	ppm	7/5/7783	79.0	I	NR	NR	NR	NR	NR	6.60E-01	4.40E-01	3.30E-01	2.00E-01	1.50E-01	2.20E+00	1.40E+00	1.10E+00	6.50E-01	4.90E-01
132	Hydrogensulfide	ppm	7783-06-4	34.1	F	7.50E-01	6.00E-01	5.10E-01	3.60E-01	3.30E-01	4.10E+01	3.20E+01	2.70E+01	2.00E+01	1.70E+01	7.60E+01	5.90E+01	5.00E+01	3.70E+01	3.10E+01
133	Iron pentacarbonyl	ppm	13463-40-6	195.9	F	NR	NR	NR	NR	NR	7.70E-02	7.70E-02	6.00E-02	3.70E-02	2.50E-02	2.30E-01	2.30E-01	1.80E-01	1.10E-01	7.50E-02
134	Isobutyl chloroformate	ppm	543-27-1	136.6	I	NR	NR	NR	NR	NR	4.00E+00	2.80E+00	2.20E+00	5.70E-01	2.80E-01	1.20E+01	8.40E+00	6.70E+00	1.70E+00	8.30E-01
135	Isobutyronitrile	ppm	78-82-0	69.1	I	NR	NR	NR	NR	NR	3.30E+01	2.30E+01	1.80E+01	1.10E+01	7.50E+00	1.20E+02	8.50E+01	6.80E+01	1.70E+01	8.50E+00

Table 1 (4 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
136	Isopropyl-chloroformate	ppm	108-23-6	122.6	I	NR	NR	NR	NR	NR	6.00E+00	4.30E+00	3.30E+00	8.30E-01	4.30E-01	1.80E+01	1.30E+01	1.00E+01	2.50E+00	1.30E+00
137	Jet Fuels (JP-5 & 8)	mg/m^3	-20-6, 70892-	212.4	F	3.63E+01	3.63E+01	3.63E+01	3.63E+01	3.63E+01	1.38E+02	1.38E+02	1.38E+02	1.38E+02	1.38E+02	NR	NR	NR	NR	NR
138	Ketene	ppm	463-51-4	42.0	I	2.40E-01	2.40E-01	1.90E-01	1.20E-01	8.80E-02	8.30E-01	8.30E-01	6.60E-01	4.20E-01	2.30E-01	2.50E+00	2.50E+00	2.00E+00	1.20E+00	6.80E-01
139	Lewisite 1 mixtures with Lewisite 3	mg/m^3	40334-70-1	207.3	I	NR	NR	NR	NR	NR	7.67E-02	2.71E-02	1.42E-02	4.13E-03	2.12E-03	4.60E-01	1.65E-01	8.73E-02	2.48E-02	1.30E-02
140	Lewisite 1 mixtures with Lewisite 2	mg/m^3	40334-69-8	207.3	I	NR	NR	NR	NR	NR	7.67E-02	2.71E-02	1.42E-02	4.13E-03	2.12E-03	4.60E-01	1.65E-01	8.73E-02	2.48E-02	1.30E-02
141	Lewisite 1	mg/m^3	541-25-3	207.3	I	NR	NR	NR	NR	NR	7.67E-02	2.71E-02	1.42E-02	4.13E-03	2.12E-03	4.60E-01	1.65E-01	8.73E-02	2.48E-02	1.30E-02
142	Magnesium aluminum phosphide	ppm	NA	82.3	F	NR	NR	NR	NR	NR	1.30E+00	1.3	6.70E-01	1.70E-01	8.00E-02	2.40E+00	2.40E+00	1.20E+00	3.00E-01	1.50E-01
143	Magnesium Phosphide	ppm	12057-74-8	134.9	F	NR	NR	NR	NR	NR	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	3.60E+00	3.60E+00	1.80E+00	4.50E-01	2.30E-01
144	Malathion	mg/m^3	121-75-5	330.4	I	1.11E+00	1.11E+00	1.11E+00	1.11E+00	1.11E+00	1.11E+01	1.11E+01	8.89E+00	5.70E+00	3.70E+00	3.70E+01	3.70E+01	2.89E+01	1.85E+01	1.04E+01
145	Malononitrile	ppm	109-77-3	66.1	I	NR	NR	NR	NR	NR	7.50E+00	7.50E+00	4.90E+00	2.00E+00	1.30E+00	1.50E+01	1.50E+01	1.00E+01	4.30E+00	2.80E+00
146	Mercury Vapor	mg/m^3	7439-97-6	200.6	I	NR	NR	NR	NR	NR	3.78E-01	2.56E-01	2.07E-01	8.17E-02	4.02E-02	1.95E+00	1.34E+00	1.09E+00	2.68E-01	2.68E-01
147	Methacrylaldehyde	ppm	78-85-3	70.1	I	2.00E-01	2.00E-01	2.00E-01	2.00E-01	2.00E-01	3.50E+00	3.50E+00	2.80E+00	1.80E+00	1.10E+00	5.90E+00	5.90E+00	4.70E+00	2.90E+00	1.90E+00
148	Methacrylicacid	ppm	79-41-4	86.1	I	6.70E+00	6.70E+00	6.70E+00	6.70E+00	6.70E+00	7.60E+01	7.60E+01	6.10E+01	3.80E+01	2.50E+01	2.80E+02	2.80E+02	2.20E+02	1.40E+02	7.10E+01
149	Methacrylonitrile	ppm	126-98-7	67.1	I	2.00E+00	2.00E+00	1.00E+00	1.00E+00	1.00E+00	1.60E+01	1.60E+01	1.30E+01	6.50E+00	6.50E+00	3.20E+01	3.20E+01	2.50E+01	1.30E+01	1.30E+01
150	Methamidophos	mg/m^3	10265-92-6	141.1	P	4.16E-01	4.16E-01	3.29E-01	2.08E-01	1.06E-01	7.80E-01	7.80E-01	6.24E-01	3.99E-01	1.91E-01	1.73E+00	1.73E+00	1.40E+00	8.84E-01	4.33E-01
151	Methanol	ppm	67-56-1	32.0	I	6.70E+02	6.70E+02	5.30E+02	3.40E+02	2.70E+02	1.10E+04	4.00E+03	2.10E+03	7.30E+02	5.20E+02	4.00E+04	1.40E+04	7.20E+03	2.40E+03	1.60E+03
152	Methan-sulfonylchloride	ppm	124-63-0	114.5	I	NR	NR	NR	NR	NR	4.00E+00	4.00E+00	2.10E+00	5.30E-01	2.60E-01	1.20E+01	1.20E+01	6.20E+00	1.60E+00	7.80E-01
153	Methomyl	mg/m^3	16752-77-5	162.2	P	NR	NR	NR	NR	NR	1.06E+00	1.06E+00	8.60E-01	4.98E-01	2.56E-01	3.17E+00	3.17E+00	2.56E+00	1.51E+00	7.84E-01
154	Methyl dichloroarsine	mg/m^3	593-89-5	160.9	I	NR	NR	NR	NR	NR	9.58E-02	2.13E-02	8.06E-03	2.28E-03	9.58E-04	2.89E-01	6.39E-02	2.43E-02	6.69E-03	2.89E-03
155	Methyl isocyanate	ppm	624-83-9	57.1	F	NR	NR	NR	NR	NR	4.00E-01	1.30E-01	6.70E-02	1.70E-02	8.00E-03	1.20E+00	4.00E-01	2.00E-01	5.00E-02	2.50E-02
156	Methyl isothiocyanate	ppm	75-09-2	84.9	I	2.90E+02	2.30E+02	2.00E+02	NR	NR	1.70E+03	1.20E+03	5.60E+02	1.00E+02	6.00E+01	1.20E+04	8.50E+03	6.90E+03	4.90E+03	2.10E+03
157	Methyl nonafluorobutyl ether	ppm	-07-6and1637	162.2	F	2.50E+03	2.50E+03	2.50E+03	2.50E+03	2.50E+03	8.20E+03	8.20E+03	8.20E+03	8.20E+03	8.20E+03	1.50E+04	1.50E+04	1.50E+04	1.50E+04	1.50E+04
158	Methyl nonafluoroisobutyl	ppm	-07-6and1637	162.2	F	2.50E+03	2.50E+03	2.50E+03	2.50E+03	2.50E+03	8.20E+03	8.20E+03	8.20E+03	8.20E+03	8.20E+03	1.50E+04	1.50E+04	1.50E+04	1.50E+04	1.50E+04
159	Methyl parathion	mg/m^3	298-00-0	263.2	I	NR	NR	NR	NR	NR	1.95E-01	1.39E-01	1.12E-01	6.78E-02	3.44E-02	5.95E-01	4.09E-01	3.25E-01	2.04E-01	1.02E-01
160	Methylamine	ppm	74-89-5	31.1	I	1.50E+01	1.50E+01	1.50E+01	1.50E+01	1.50E+01	1.60E+02	9.20E+01	6.40E+01	3.10E+01	2.10E+01	9.10E+02	5.10E+02	3.50E+02	1.70E+02	1.10E+02
161	Methylbromide	ppm	74-83-9	94.9	I	NR	NR	NR	NR	NR	9.40E+02	3.80E+02	2.10E+02	6.70E+01	6.70E+01	3.30E+03	1.30E+03	7.40E+02	2.30E+02	1.30E+02
162	Methylchloride	ppm	74-87-3	50.5	I	NR	NR	NR	NR	NR	1.10E+03	1.10E+03	9.10E+02	5.70E+02	3.80E+02	3.80E+03	3.80E+03	3.00E+03	1.90E+03	1.30E+03
163	Methylchloroformate	ppm	79-22-1	94.5	I	NR	NR	NR	NR	NR	4.00E+00	2.80E+00	2.20E+00	1.40E+00	7.00E-01	1.20E+01	8.50E+00	6.70E+00	4.20E+00	2.10E+00
164	Methylchlorosilane	ppm	993-00-0	80.6	I	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.00E+02	4.30E+01	2.20E+01	1.10E+01	1.10E+01	6.20E+02	2.10E+02	1.00E+02	2.60E+01	2.60E+01
165	Methyldichlorosilane	ppm	75-54-7	114.0	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
166	Methylene chloride	ppm	556-61-6	73.1	I	8.00E-01	8.00E-01	8.00E-01	8.00E-01	8.00E-01	4.30E+01	2.90E+01	2.30E+01	9.00E+00	4.30E+00	1.30E+02	8.80E+01	7.00E+01	2.70E+01	1.30E+01
167	Methyl-ethyl-ketone	ppm	78-93-3	72.1	F	2.00E+02	2.00E+02	2.00E+02	2.00E+02	2.00E+02	4.90E+03	3.40E+03	2.70E+03	1.70E+03	1.70E+03	1.00E+04	1.00E+04	4.00E+03	2.50E+03	2.50E+03
168	Methylhydrazine	ppm	60-34-4	46.1	F	NR	NR	NR	NR	NR	5.30E+00	1.80E+00	9.00E-01	2.30E-01	1.10E-01	1.60E+01	5.50E+00	2.70E+00	6.80E-01	3.40E-01
169	Methyliodide	ppm	74-88-4	141.9	P	5.40E+01	3.10E+01	2.20E+01	1.10E+01	1.10E+01	2.00E+02	1.20E+02	8.20E+01	4.10E+01	2.90E+01	6.70E+02	4.00E+02	2.90E+02	1.50E+02	9.80E+01
170	Methylmercaptan	ppm	74-93-1	48.1	I	NR	NR	NR	NR	NR	5.90E+01	5.90E+01	4.70E+01	3.00E+01	1.90E+01	1.20E+02	8.60E+01	6.80E+01	4.30E+01	2.20E+01

Table 1 (5 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
171	Methylmethacrylate	ppm	80-62-6	100.1	I	1.70E+01	1.70E+01	1.70E+01	1.70E+01	1.70E+01	1.50E+02	1.50E+02	1.20E+02	7.60E+01	5.00E+01	7.20E+02	7.20E+02	5.70E+02	3.60E+02	1.80E+02
172	Methyl-tertiary-butylether(MTBE)	ppm	1634-04-4	88.1	I	5.00E+01	5.00E+01	5.00E+01	5.00E+01	5.00E+01	1.40E+03	8.00E+02	5.70E+02	4.00E+02	4.00E+02	1.30E+04	7.50E+03	5.30E+03	2.70E+03	1.90E+03
173	Methylvinyl-dichlorosilane	ppm	124-70-9	141.1	I	9.00E-01	9.00E-01	9.00E-01	9.00E-01	9.00E-01	5.00E+01	2.20E+01	1.10E+01	5.50E+00	5.50E+00	3.10E+02	1.10E+02	5.00E+01	1.30E+01	1.30E+01
174	Methylvinylketone	ppm	78-94-4	70.1	I	1.70E-01	1.70E-01	1.70E-01	1.70E-01	1.70E-01	1.50E+00	1.50E+00	1.20E+00	7.60E-01	5.00E-01	3.10E+00	3.10E+00	2.40E+00	1.50E+00	1.00E+00
175	Monochloro-aceticacid	ppm	79-11-8	94.5	F	NR	NR	NR	NR	NR	1.20E+01	8.30E+00	6.60E+00	1.70E+00	8.30E-01	NR	NR	NR	NR	NR
176	Monocrotophos	mg/m^3	6923-22-4	223.2	P	NR	NR	NR	NR	NR	4.71E-02	3.40E-02	2.63E-02	2.30E-02	1.10E-02	1.42E-01	1.01E-01	8.00E-02	6.79E-02	3.40E-02
177	N,N-Dimethylformamide	ppm	68-12-2	73.1	F	NR	NR	NR	NR	NR	1.10E+02	1.10E+02	9.10E+01	5.70E+01	3.80E+01	9.70E+02	6.70E+02	5.30E+02	2.80E+02	1.40E+02
178	n-Butylacrylate	ppm	141-32-2	128.2	I	8.30E+00	8.30E+00	8.30E+00	8.30E+00	8.30E+00	1.60E+02	1.60E+02	1.30E+02	8.10E+01	5.30E+01	8.20E+02	8.20E+02	4.80E+02	1.70E+02	9.70E+01
179	n-Butylchloroformate	ppm	592-34-7	136.6	I	NR	NR	NR	NR	NR	4.00E+00	2.80E+00	2.20E+00	5.70E-01	2.80E-01	1.20E+01	8.40E+00	6.70E+00	1.70E+00	8.30E-01
180	n-Butylisocyanate	ppm	111-36-4	99.1	I	1.30E-02	1.30E-02	1.30E-02	1.30E-02	1.30E-02	2.30E-02	2.30E-02	2.30E-02	2.30E-02	2.30E-02	3.10E-01	3.10E-01	2.50E-01	1.50E-01	8.00E-02
181	Nerve Agent GA (Tabun)	ppm	77-81-6	162.1	F	1.00E-03	6.00E-04	4.20E-04	2.10E-04	1.50E-04	1.30E-02	7.50E-03	5.30E-03	2.60E-03	2.00E-03	1.10E-01	5.70E-02	3.90E-02	2.10E-02	1.50E-02
182	Nickel carbonyl	ppm	13463-39-3	170.7	F	NR	NR	NR	NR	NR	1.00E-01	7.20E-02	3.60E-02	9.00E-03	4.50E-03	4.60E-01	3.20E-01	1.60E-01	4.00E-02	2.00E-02
183	Nitric Acid	ppm	7697-37-2	63.0	I	5.30E-01	5.30E-01	5.30E-01	5.30E-01	5.30E-01	4.30E+01	3.00E+01	2.40E+01	6.00E+00	3.00E+00	1.70E+02	1.20E+02	9.20E+01	2.30E+01	1.10E+01
184	Nitric Oxide	ppm	10102-43-9	31.0	I	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR
185	Nitrogen dioxide	ppm	10102-44-0	46.0	I	5.00E-01	5.00E-01	5.00E-01	5.00E-01	5.00E-01	2.00E+01	1.50E+01	1.20E+01	8.20E+00	6.70E+00	3.40E+01	2.50E+01	2.00E+01	1.40E+01	1.10E+01
186	Nitrogen Mustard- 3	mg/m^3	555-77-1	241.0	I	NR	NR	NR	NR	NR	1.56E-02	5.27E-03	2.63E-03	6.71E-04	3.35E-04	2.63E-01	8.86E-02	4.43E-02	1.11E-02	5.63E-03
187	Nitrogen mustard-1	mg/m^3	538-07-8	170.1	I	NR	NR	NR	NR	NR	1.87E-02	6.34E-03	3.17E-03	8.07E-04	4.03E-04	3.17E-01	1.07E-01	5.33E-02	1.34E-02	6.77E-03
188	Nitrogen Mustard-2	mg/m^3	51-75-2	156.1	I	NR	NR	NR	NR	NR	2.04E-02	6.91E-03	3.45E-03	8.79E-04	4.40E-04	3.45E-01	1.16E-01	5.81E-02	1.46E-02	7.38E-03
189	Nitrogen Tetroxide	mg/m^3	10544-72-6	92.0	I	2.54E-01	2.54E-01	2.54E-01	2.54E-01	2.54E-01	1.03E+01	7.57E+00	6.22E+00	4.05E+00	3.51E+00	1.73E+01	1.27E+01	1.03E+01	7.03E+00	5.68E+00
190	Nitrogen trifluoride	ppm	7783-54-2	71.0	I	1.20E+03	4.00E+02	2.00E+02	5.00E+01	2.50E+01	3.10E+03	1.10E+03	5.30E+02	1.40E+02	6.80E+01	5.00E+03	1.70E+03	8.60E+02	2.20E+02	1.10E+02
191	Nonyltrichlorosilane	ppm	5283-67-0	261.7	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
192	Octadecyltrichlorosilane	ppm	112-04-9	387.9	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
193	Octyltrichlorosilane	ppm	5283-66-9	247.7	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
194	Oleum	mg/m^3	8014-95-7	178.1	I	2.75E-02	2.75E-02	2.75E-02	2.75E-02	2.75E-02	1.19E+00	1.19E+00	1.19E+00	1.19E+00	1.19E+00	3.71E+01	2.75E+01	2.20E+01	1.51E+01	1.28E+01
195	Osmiumtetroxide	ppm	20816-12-0	254.2	I	NR	NR	NR	NR	NR	1.50E-02	1.10E-02	8.40E-03	3.30E-03	1.70E-03	5.00E+00	5.00E+00	4.00E+00	2.50E+00	2.00E+00
196	Otto Fuel (mainly Propylene Glycol)	ppm	106602-80-6	166.1	F	3.30E-01	3.30E-01	1.70E-01	5.00E-02	3.00E-02	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	1.60E+01	1.60E+01	1.30E+01	8.00E+00	5.30E+00
197	Oxamyl	mg/m^3	23135-22-0	219.3	P	4.01E-01	2.01E-01	1.34E-01	5.46E-02	3.57E-02	5.91E-01	3.01E-01	2.01E-01	8.14E-02	5.24E-02	1.78E+00	9.14E-01	5.91E-01	2.45E-01	1.56E-01
198	Oxygendifluoride	ppm	7783-41-7	54.0	I	NR	NR	NR	NR	NR	4.30E+00	1.60E+00	8.30E-01	2.40E-01	1.30E-01	1.30E+01	4.70E+00	2.50E+00	7.10E-01	3.80E-01
199	Parathion	mg/m^3	56-38-2	291.3	I	NR	NR	NR	NR	NR	2.35E-01	1.60E-01	1.26E-01	8.07E-02	4.03E-02	3.03E-01	2.10E-01	1.68E-01	1.09E-01	5.29E-02
200	Pentaborane	ppm	19624-22-7	63.1	I	NR	NR	NR	NR	NR	5.60E-01	2.40E-01	1.40E-01	4.80E-02	2.80E-02	2.80E+00	1.20E+00	7.00E-01	2.40E-01	1.40E-01
201	Peracetic Acid	mg/m^3	79-21-0	76.1	F	1.71E-01	1.71E-01	1.71E-01	1.71E-01	1.71E-01	5.26E-01	5.26E-01	5.26E-01	5.26E-01	5.26E-01	1.97E+01	9.87E+00	4.93E+00	2.07E+00	1.35E+00
202	Perchloro-methylmercaptan	ppm	594-42-3	185.9	F	1.30E-02	1.30E-02	1.30E-02	1.30E-02	1.30E-02	5.30E-01	3.70E-01	3.00E-01	7.70E-02	3.70E-02	1.60E+00	1.10E+00	9.00E-01	2.30E-01	1.10E-01
203	Perchlorylfluoride	ppm	7616-94-6	102.4	I	1.80E+00	1.80E+00	1.50E+00	9.20E-01	6.00E-01	5.00E+00	5.00E+00	4.00E+00	2.50E+00	1.20E+00	1.50E+01	1.50E+01	1.20E+01	7.50E+00	3.70E+00
204	Perfluoroisobutylene	ppm	382-21-8	200.0	I	NR	NR	NR	NR	NR	6.70E-01	2.20E-01	1.10E-01	2.80E-02	1.40E-02	2.00E+00	6.70E-01	3.30E-01	8.30E-02	4.20E-02
205	Phenol	ppm	108-95-2	94.1	F	1.90E+01	1.90E+01	1.50E+01	9.50E+00	6.30E+00	2.90E+01	2.90E+01	2.30E+01	1.50E+01	1.20E+01	NR	NR	NR	NR	NR

Table 1 (6 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
206	Phenyl dichloroarsine	mg/m^3	696-28-6	222.9	I	NR	NR	NR	NR	NR	4.06E-02	1.32E-02	6.69E-03	NR	NR	1.21E-01	4.06E-02	1.98E-02	NR	NR
207	Phenylchloroformate	ppm	1885-14-9	156.6	I	NR	NR	NR	NR	NR	2.40E-01	2.40E-01	1.90E-01	1.20E-01	6.00E-02	7.20E-01	7.20E-01	5.70E-01	3.60E-01	1.80E-01
208	Phenylisocyanate	ppm	103-71-9	119.1	I	2.00E-02	2.00E-02	2.00E-02	2.00E-02	2.00E-02	1.80E-01	1.80E-01	1.50E-01	9.20E-02	6.00E-02	3.00E-01	3.00E-01	2.40E-01	1.50E-01	7.50E-02
209	PhenylMercaptan	ppm	108-98-5	110.2	I	NR	NR	NR	NR	NR	1.00E+00	7.00E-01	5.30E-01	3.30E-01	1.70E-01	3.00E+00	2.10E+00	1.60E+00	1.00E+00	5.20E-01
210	Phenyltrichlorosilane	ppm	98-13-5	211.6	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
211	Phorate	mg/m^3	298-02-2	260.4	I	NR	NR	NR	NR	NR	6.89E-03	4.72E-03	3.77E-03	9.43E-04	4.72E-04	2.08E-02	1.42E-02	1.13E-02	2.92E-03	1.42E-03
212	Phosgene	ppm	75-44-5	98.9	F	NR	NR	NR	NR	NR	6.00E-01	6.00E-01	3.00E-01	8.00E-02	4.00E-02	3.60E+00	1.50E+00	7.50E-01	2.00E-01	9.00E-02
213	Phosgene oxime	mg/m^3	1794-86-1	113.9	I	3.65E-02	1.20E-02	6.01E-03	1.48E-03	7.51E-04	1.07E-01	3.65E-02	1.78E-02	4.51E-03	2.15E-03	7.73E+00	5.36E+00	2.79E+00	6.65E-01	3.43E-01
214	Phosphamidon	mg/m^3	13171-21-6	299.7	P	NR	NR	NR	NR	NR	3.02E-02	3.02E-02	2.45E-02	1.55E-02	7.59E-03	8.97E-02	8.97E-02	7.34E-02	4.65E-02	2.28E-02
215	Phosphine	ppm	7803-51-2	34.0	F	NR	NR	NR	NR	NR	4.00E+00	4.00E+00	2.00E+00	5.00E-01	2.50E-01	7.20E+00	7.20E+00	3.60E+00	9.00E-01	4.50E-01
216	Phosphorus oxychloride	ppm	10025-87-3	153.3	F	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	1.10E+00	1.10E+00	8.50E-01	5.40E-01	2.70E-01
217	Phosphorus trichloride	ppm	7719-12-2	137.3	F	3.40E-01	3.40E-01	3.40E-01	3.40E-01	3.40E-01	2.50E+00	2.50E+00	2.00E+00	1.30E+00	8.30E-01	7.00E+00	7.00E+00	5.60E+00	3.50E+00	1.80E+00
218	Piperidine	ppm	110-89-4	85.1	I	1.00E+01	1.00E+01	6.60E+00	2.60E+00	1.70E+00	5.00E+01	5.00E+01	3.30E+01	1.30E+01	8.30E+00	3.70E+02	1.80E+02	1.10E+02	4.50E+01	2.80E+01
219	Potassium cyanide	mg/m^3	151-50-8	65.1	I	2.44E+00	2.44E+00	1.96E+00	1.30E+00	1.00E+00	1.67E+01	1.00E+01	7.04E+00	3.44E+00	2.44E+00	2.67E+01	2.07E+01	1.48E+01	8.52E+00	6.67E+00
220	Potassium Phosphide	ppm	20770-41-6	150.3	F	NR	NR	NR	NR	NR	4.00E+00	4.00E+00	2.00E+00	5.00E-01	2.50E-01	7.20E+00	7.20E+00	3.60E+00	9.00E-01	4.50E-01
221	Propane	ppm	74-98-6	44.1	I	1.00E+04	6.90E+03	5.50E+03	5.50E+03	5.50E+03	1.70E+04	1.70E+04	1.70E+04	1.70E+04	1.70E+04	3.30E+04	3.30E+04	3.30E+04	3.30E+04	3.30E+04
222	Propargyl alcohol	ppm	107-19-7	56.1	I	2.50E+00	2.50E+00	2.50E+00	2.50E+00	2.50E+00	2.00E+01	2.00E+01	1.60E+01	1.00E+01	6.60E+00	1.30E+02	9.10E+01	7.20E+01	2.90E+01	1.40E+01
223	Propionaldehyde	ppm	123-38-6	58.1	I	4.50E+01	4.50E+01	4.50E+01	4.50E+01	4.50E+01	3.30E+02	3.30E+02	2.60E+02	1.70E+02	1.10E+02	1.10E+03	1.10E+03	8.40E+02	5.30E+02	2.60E+02
224	Propionitrile	ppm	107-12-0	55.1	I	NR	NR	NR	NR	NR	9.00E+00	9.00E+00	7.00E+00	2.90E+00	1.40E+00	4.60E+01	4.60E+01	3.70E+01	2.30E+01	1.20E+01
225	Propylchloroformate	ppm	109-61-5	122.6	I	NR	NR	NR	NR	NR	6.70E+00	4.70E+00	3.70E+00	9.00E-01	4.70E-01	2.00E+01	1.40E+01	1.10E+01	2.70E+00	1.40E+00
226	Propylene glycoldinitrate	ppm	6423-43-4	166.1	F	3.30E-01	3.30E-01	1.70E-01	5.00E-02	3.00E-02	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	1.60E+01	1.60E+01	1.30E+01	8.00E+00	5.30E+00
227	Propyleneimine	ppm	75-55-8	57.1	F	NR	NR	NR	NR	NR	8.30E+01	2.50E+01	1.20E+01	2.50E+00	1.20E+00	1.70E+02	5.00E+01	2.30E+01	5.10E+00	2.40E+00
228	Propyleneoxide	ppm	75-56-9	58.1	F	7.30E+01	7.30E+01	7.30E+01	7.30E+01	7.30E+01	4.40E+02	4.40E+02	2.90E+02	1.30E+02	8.60E+01	1.30E+03	1.30E+03	8.70E+02	3.90E+02	2.60E+02
229	Propyltri-chlorosilane	ppm	141-57-1	177.5	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
230	Red Phosphorus	mg/m^3	7723-14-0	31.0	P	1.32E+00	9.28E-01	7.31E-01	1.84E-01	9.28E-02	3.95E+00	2.76E+00	2.17E+00	5.53E-01	2.76E-01	1.68E+01	1.17E+01	9.28E+00	2.37E+00	1.17E+00
231	sec-Butylchloroformate	ppm	17462-58-7	136.6	I	NR	NR	NR	NR	NR	4.00E+00	2.80E+00	2.20E+00	5.70E-01	2.80E-01	1.20E+01	8.40E+00	6.70E+00	1.70E+00	8.30E-01
232	Seleniumhexafluoride	ppm	7783-79-1	193.0	I	6.70E-02	6.70E-02	5.30E-02	3.30E-02	1.70E-02	1.10E-01	1.10E-01	8.70E-02	5.70E-02	2.80E-02	3.30E-01	3.30E-01	2.60E-01	1.70E-01	8.30E-02
233	Silane	ppm	7803-62-5	28.1	I	1.00E+02	1.00E+02	1.00E+02	NR	NR	1.70E+02	1.70E+02	1.30E+02	8.00E+01	4.20E+01	3.00E+02	3.00E+02	2.70E+02	1.70E+02	8.00E+01
234	Silicontetrachloride	ppm	10026-04-7	169.9	I	4.50E-01	4.50E-01	4.50E-01	4.50E-01	4.50E-01	2.50E+01	1.10E+01	5.50E+00	2.80E+00	2.80E+00	1.60E+02	5.30E+01	2.50E+01	6.50E+00	6.50E+00
235	Silicontetrafluoride	ppm	7783-61-1	104.1	I	5.00E-02	5.00E-02	5.00E-02	5.00E-02	5.00E-02	6.30E+00	4.30E+00	3.30E+00	8.70E-01	4.30E-01	1.90E+01	1.30E+01	1.00E+01	2.60E+00	1.30E+00
236	Sodium cyanide	mg/m^3	143-33-9	49.0	I	2.50E+00	2.50E+00	2.00E+00	1.30E+00	1.00E+00	1.70E+01	1.00E+01	7.00E+00	3.50E+00	2.50E+00	2.70E+01	2.10E+01	1.50E+01	8.50E+00	6.50E+00
237	Sodium Phosphide	ppm	12058-85-4	99.9	F	NR	NR	NR	NR	NR	4.00E+00	4.00E+00	2.00E+00	5.00E-01	2.50E-01	7.20E+00	7.20E+00	3.60E+00	9.00E-01	4.50E-01
238	Stibine	ppm	7803-52-3	121.8	I	NR	NR	NR	NR	NR	4.20E+00	2.90E+00	1.50E+00	3.60E-01	1.80E-01	2.80E+01	1.90E+01	9.60E+00	2.40E+00	1.20E+00
239	Strontium phosphide	ppm	12504-13-1	324.8	F	NR	NR	NR	NR	NR	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	3.60E+00	3.60E+00	1.80E+00	4.50E-01	2.30E-01
240	Styrene	ppm	100-42-5	104.2	I	2.00E+01	2.00E+01	2.00E+01	2.00E+01	2.00E+01	2.30E+02	1.60E+02	1.30E+02	1.30E+02	1.30E+02	1.90E+03	1.90E+03	1.10E+03	3.40E+02	3.40E+02

Table 1 (7 of 8)

n	Chemical	Units	CAS #	MW	Stage	AEGL-1 (1/6h)	AEGL-1 (1/2h)	AEGL-1 (1h)	AEGL-1 (4h)	AEGL-1 (8h)	AEGL-2 (1/6h)	AEGL-2 (1/2h)	AEGL-2 (1h)	AEGL-2 (4h)	AEGL-2 (8h)	AEGL-3 (1/6h)	AEGL-3 (1/2h)	AEGL-3 (1h)	AEGL-3 (4h)	AEGL-3 (8h)
241	Sulfur dioxide	ppm	7446-09-5	64.1	F	2.00E-01	2.00E-01	2.00E-01	2.00E-01	2.00E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	7.50E-01	3.00E+01	3.00E+01	3.00E+01	1.90E+01	9.60E+00
242	Sulfur mustard	ppm	505-60-2	159.1	F	6.00E-02	2.00E-02	1.00E-02	3.00E-03	1.00E-03	9.00E-02	3.00E-02	2.00E-02	4.00E-03	2.00E-03	5.90E-01	4.10E-01	3.20E-01	8.00E-02	4.00E-02
243	Sulfur trioxide	mg/m^3	7446-11-9	80.1	I	6.11E-02	6.11E-02	6.11E-02	6.11E-02	6.11E-02	2.66E+00	2.66E+00	2.66E+00	2.66E+00	2.66E+00	8.25E+01	6.11E+01	4.89E+01	3.36E+01	2.84E+01
244	Sulfuric acid	mg/m^3	7664-93-9	98.1	I	4.90E-02	4.90E-02	4.90E-02	4.90E-02	4.90E-02	2.13E+00	2.13E+00	2.13E+00	2.13E+00	2.13E+00	6.62E+01	4.90E+01	3.92E+01	2.70E+01	2.28E+01
245	Sulfuryl chloride	ppm	7791-25-5	135.0	F	NR	NR	NR	NR	NR	4.70E+00	4.70E+00	3.70E+00	2.30E+00	1.20E+00	1.40E+01	1.40E+01	1.10E+01	7.00E+00	3.50E+00
246	Sulfuryl fluoride	ppm	2699-79-8	102.1	I	NR	NR	NR	NR	NR	2.70E+01	2.70E+01	2.10E+01	1.30E+01	6.70E+00	8.10E+01	8.10E+01	6.40E+01	4.00E+01	2.00E+01
247	Tear Gas	mg/m^3	2698-41-1	188.6	I	6.49E-03	6.49E-03	6.49E-03	6.49E-03	6.49E-03	6.49E-02	6.49E-02	6.49E-02	6.49E-02	6.49E-02	1.82E+01	3.76E+00	1.43E+00	1.95E-01	1.95E-01
248	Tellurium hexafluoride	ppm	7783-80-4	241.6	I	NR	NR	NR	NR	NR	3.20E-02	2.20E-02	1.80E-02	1.10E-02	5.70E-03	9.60E-02	6.70E-02	5.30E-02	3.30E-02	1.70E-02
249	Tetrachloroethylene	ppm	127-18-4	165.8	I	3.50E+01	3.50E+01	3.50E+01	3.50E+01	3.50E+01	2.30E+02	2.30E+02	2.30E+02	1.20E+02	8.10E+01	1.60E+03	1.60E+03	1.20E+03	5.80E+02	4.10E+02
250	Tetrafluoroethylene	ppm	116-14-3	100.0	I	2.70E+02	2.70E+02	2.20E+02	1.40E+02	9.00E+01	6.90E+02	6.90E+02	5.50E+02	3.40E+02	2.30E+02	4.20E+03	4.20E+03	3.30E+03	2.10E+03	1.00E+03
251	Tetramethoxysilane	ppm	681-84-5	152.2	I	NR	NR	NR	NR	NR	1.10E+00	1.10E+00	9.10E-01	5.70E-01	3.80E-01	1.70E+00	1.70E+00	1.40E+00	8.70E-01	4.30E-01
252	Tetranitromethane	ppm	509-14-8	196.0	F	NR	NR	NR	NR	NR	6.60E-01	6.60E-01	5.20E-01	3.30E-01	1.70E-01	2.20E+00	2.20E+00	1.70E+00	1.10E+00	5.50E-01
253	Thionylchloride	ppm	9/7/7719	119.0	I	NR	NR	NR	NR	NR	4.30E+00	3.00E+00	2.40E+00	5.90E-01	3.00E-01	2.50E+01	1.70E+01	1.40E+01	3.40E+00	1.70E+00
254	Titanium tetrachloride	ppm	7550-45-0	189.7	I	NR	NR	NR	NR	NR	7.60E+00	2.20E+00	1.00E+00	2.10E-01	9.40E-02	3.80E+01	1.30E+01	5.70E+00	2.00E+00	9.10E-01
255	t-Octylmercaptan	ppm	141-59-3	146.3	I	NR	NR	NR	NR	NR	7.70E-01	7.70E-01	6.00E-01	4.00E-01	1.90E-01	2.30E+00	2.30E+00	1.80E+00	1.20E+00	5.80E-01
256	Toluene	ppm	108-88-3	92.1	I	2.00E+02	2.00E+02	2.00E+02	2.00E+02	2.00E+02	3.10E+03	1.60E+03	1.20E+03	7.90E+02	6.50E+02	1.30E+04	6.10E+03	4.50E+03	3.00E+03	2.50E+03
257	trans-1,2-Dichloroethylene	ppm	156-60-5	96.9	F	2.80E+02	2.80E+02	2.80E+02	2.80E+02	2.80E+02	1.00E+03	1.00E+03	1.00E+03	6.90E+02	4.50E+02	1.70E+03	1.70E+03	1.70E+03	1.20E+03	6.20E+02
258	trans-Crotonaldehyde	ppm	123-73-9	70.1	F	1.90E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01	2.70E+01	8.90E+00	4.40E+00	1.10E+00	5.60E-01	4.40E+01	2.70E+01	1.40E+01	2.60E+00	1.50E+00
259	Trichloroethylene	ppm	79-01-6	131.4	I	2.60E+02	1.80E+02	1.30E+02	8.40E+01	7.70E+01	9.60E+02	6.20E+02	4.50E+02	2.70E+02	2.40E+02	6.10E+03	6.10E+03	3.80E+03	1.50E+03	9.70E+02
260	Trichloromethylsilane	ppm	75-79-6	149.5	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
261	Trichlorosilane	ppm	10025-78-2	134.4	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
262	Trifluorochloroethylene	ppm	79-38-9	116.5	I	2.90E+01	2.00E+01	1.60E+01	1.00E+01	1.00E+01	1.60E+02	1.10E+02	8.60E+01	5.40E+01	5.40E+01	1.50E+03	6.90E+02	4.20E+02	1.50E+02	9.10E+01
263	Trimethoxysilane	ppm	2487-90-3	121.2	I	NR	NR	NR	NR	NR	2.90E+00	1.40E+00	8.30E-01	3.30E-01	2.00E-01	8.80E+00	4.10E+00	2.50E+00	9.80E-01	6.10E-01
264	Trimethylacetylchloride	ppm	3282-30-2	120.6	I	NR	NR	NR	NR	NR	6.70E-01	6.70E-01	5.30E-01	3.30E-01	2.20E-01	2.00E+00	2.00E+00	1.60E+00	9.90E-01	6.50E-01
265	Trimethylamine	ppm	75-50-3	59.1	I	8.00E+00	8.00E+00	8.00E+00	8.00E+00	8.00E+00	2.40E+02	1.50E+02	1.20E+02	6.70E+01	5.10E+01	7.50E+02	4.90E+02	3.80E+02	2.20E+02	1.70E+02
266	Trimethylchlorosilane	ppm	75-77-4	108.6	I	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.80E+00	1.00E+02	4.30E+01	2.20E+01	1.10E+01	1.10E+01	6.20E+02	2.10E+02	1.00E+02	2.60E+01	2.60E+01
267	Trimethyl phosphite	ppm	121-45-9	124.1	I	1.10E+01	7.60E+00	6.10E+00	3.80E+00	2.50E+00	1.10E+02	7.70E+01	6.10E+01	3.80E+01	2.50E+01	5.60E+02	3.90E+02	3.10E+02	1.60E+02	8.10E+01
268	Uranium hexafluoride	mg/m^3	7783-81-5	352.0	F	2.50E-01	2.50E-01	2.50E-01	NR	NR	1.94E+00	1.32E+00	6.67E-01	1.67E-01	8.33E-02	1.50E+01	5.00E+00	2.50E+00	6.25E-01	3.13E-01
269	Vinyl acetate	ppm	108-05-4	86.1	I	6.70E+00	6.70E+00	6.70E+00	6.70E+00	6.70E+00	2.30E+02	2.30E+02	1.80E+02	1.10E+02	7.50E+01	7.60E+02	7.60E+02	6.10E+02	3.80E+02	2.50E+02
270	Vinyl chloride	ppm	75-01-4	62.5	I	4.50E+02	3.10E+02	2.50E+02	1.40E+02	7.00E+01	2.80E+03	1.60E+03	1.20E+03	8.20E+02	8.20E+02	1.20E+04	6.80E+03	4.80E+03	3.40E+03	3.40E+03
271	Vinyltrichlorosilane	ppm	75-94-5	161.5	I	6.00E-01	6.00E-01	6.00E-01	6.00E-01	6.00E-01	3.30E+01	1.40E+01	7.30E+00	3.70E+00	3.70E+00	2.10E+02	7.00E+01	3.30E+01	8.70E+00	8.70E+00
272	Xylenes	ppm	1330-20-7	106.2	F	1.30E+02	1.30E+02	1.30E+02	1.30E+02	1.30E+02	2.50E+03	1.30E+03	9.20E+02	5.00E+02	4.00E+02	7.20E+03	3.60E+03	2.50E+03	1.30E+03	1.00E+03
273	Zinc phosphide	ppm	1314-84-7	260.1	F	NR	NR	NR	NR	NR	2.00E+00	2.00E+00	1.00E+00	2.50E-01	1.30E-01	3.60E+00	3.60E+00	1.80E+00	4.50E-01	2.30E-01

Table 1 (8 of 8)

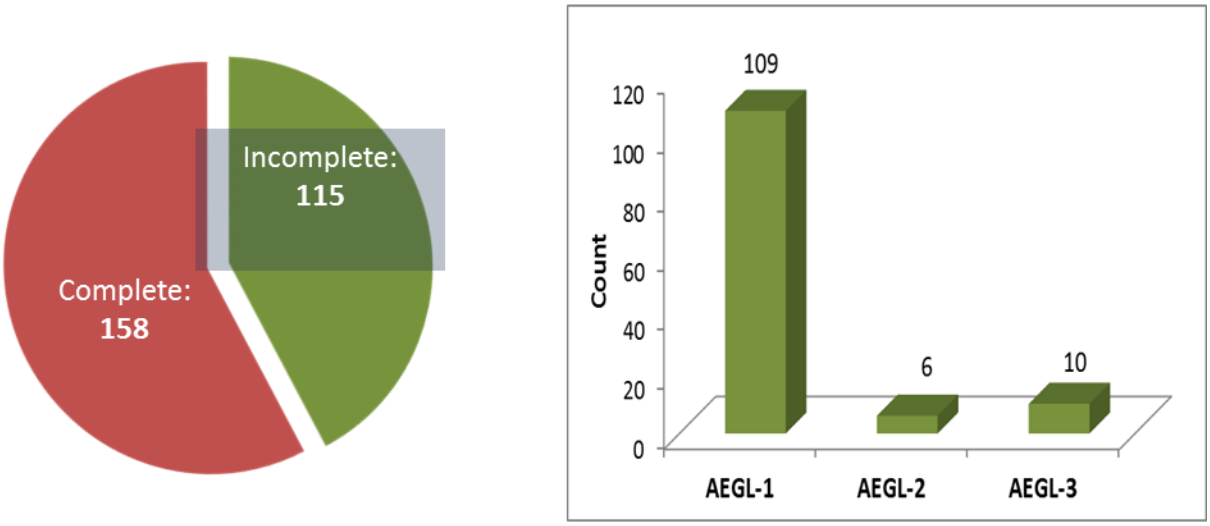


Figure 1. Frequency of unassigned AEGLs in the database. 115 (42%) compounds had at least two unassigned AEGL values. From these, 109 (91%) were concentrated in the AEGL-1 threshold. Only 6 compounds had unassigned values in the AEGL-2 threshold and 10 had unassigned values in the AEGL-3 threshold.

	Total compounds N (%)	Unassigned AEGLs N (%)	Mean	Std. Dev	Max	Min	Variance	Skewness	Variance log_{10}(AEGLs)	Skewness log_{10}(AEGLs)
AEGL-1 (1/6 h)	168 (61.5)	105 (38.5)	2.46E+02	1.27E+03	1.00E+04	5.20E-05	1.62E+06	6.89E+00	2.26E+00	6.54E-02
AEGL-1 (1/2 h)	168 (61.5)	105 (38.5)	2.01E+02	1.00E+03	8.00E+03	3.00E-05	1.00E+06	6.62E+00	2.28E+00	-5.54E-02
AEGL-1 (1 h)	168 (61.5)	105 (38.5)	1.80E+02	8.96E+02	8.00E+03	1.60E-05	8.02E+05	6.79E+00	2.32E+00	-1.32E-01
AEGL-1 (4 h)	164 (60.1)	109 (39.9)	1.78E+02	9.06E+02	8.00E+03	9.10E-06	8.21E+05	6.72E+00	2.44E+00	-2.40E-01
AEGL-1 (8 h)	164 (60.1)	109 (39.9)	1.75E+02	9.06E+02	8.00E+03	6.50E-06	8.21E+05	6.73E+00	2.51E+00	-3.02E-01
AEGL-2 (1/6 h)	270 (98.9)	3 (1.1)	5.56E+02	2.32E+03	2.40E+04	6.50E-04	5.40E+06	6.68E+00	2.12E+00	-1.00E-01
AEGL-2 (1/2 h)	270 (98.9)	3 (1.1)	4.26E+02	1.90E+03	1.70E+04	3.80E-04	3.60E+06	6.83E+00	2.16E+00	-1.30E-01
AEGL-2 (1 h)	270 (98.9)	3 (1.1)	3.80E+02	1.85E+03	1.70E+04	2.70E-04	3.43E+06	7.26E+00	2.22E+00	-7.84E-02
AEGL-2 (4 h)	267 (97.8)	6 (2.2)	3.33E+02	1.83E+03	1.70E+04	1.40E-04	3.36E+06	7.59E+00	2.36E+00	2.57E-02
AEGL-2 (8 h)	267 (97.8)	6 (2.2)	3.18E+02	1.83E+03	1.70E+04	9.50E-05	3.34E+06	7.66E+00	2.53E+00	4.14E-02
AEGL-3 (1/6 h)	264 (96.7)	9 (3.3)	1.62E+03	6.56E+03	7.70E+04	2.70E-03	4.31E+07	7.64E+00	2.01E+00	-1.05E-01
AEGL-3 (1/2 h)	264 (96.7)	9 (3.3)	1.48E+03	7.14E+03	8.60E+04	1.40E-03	5.09E+07	8.57E+00	2.02E+00	-5.66E-02
AEGL-3 (1 h)	264 (96.7)	9 (3.3)	1.30E+03	6.99E+03	8.60E+04	9.10E-04	4.88E+07	9.08E+00	2.06E+00	-9.66E-04
AEGL-3 (4 h)	261 (95.6)	12 (4.4)	1.13E+03	6.92E+03	8.60E+04	4.80E-04	4.79E+07	9.45E+00	2.15E+00	1.94E-01
AEGL-3 (8 h)	261 (95.6)	12 (4.4)	1.04E+03	6.88E+03	8.60E+04	3.50E-04	4.73E+07	9.64E+00	2.28E+00	1.90E-01

Table 2. Descriptive statistics and tests of normality for AEGLs at each exposure duration and severity health threshold. A high frequency of unassigned values existed in the AEGL-1 threshold (105 -109 compounds). Measures of central tendency include the mean, standard deviation, and the maximum and minimum for each AEGL level. Measures of normality, variance, and skewness indicated that the AEGL data was heavily right skewed. The AEGL data was normalized after log_{10} transformation.

	AEGL-1 (1/6 h)	AEGL-1 (1/2 h)	AEGL-1 (1 h)	AEGL-1 (4 h)	AEGL-1 (8 h)	AEGL-2 (1/6 h)	AEGL-2 (1/2 h)	AEGL-2 (1 h)	AEGL-2 (4 h)	AEGL-2 (8 h)	AEGL-3 (1/6 h)	AEGL-3 (1/2 h)	AEGL-3 (1 h)	AEGL-3 (4 h)	AEGL-3 (8 h)
AEGL-1 (1/6 h)	1.000	0.997	0.993	0.976	0.962	0.928	0.942	0.945	0.938	0.927	0.887	0.914	0.921	0.928	0.919
AEGL-1 (1/2 h)	0.997	1.000	0.998	0.988	0.977	0.934	0.951	0.955	0.950	0.941	0.896	0.923	0.931	0.939	0.932
AEGL-1 (1 h)	0.993	0.998	1.000	0.994	0.986	0.940	0.957	0.961	0.959	0.951	0.904	0.930	0.938	0.945	0.940
AEGL-1 (4 h)	0.976	0.988	0.994	1.000	0.998	0.944	0.962	0.968	0.973	0.969	0.912	0.938	0.946	0.954	0.952
AEGL-1 (8 h)	0.962	0.977	0.986	0.998	1.000	0.943	0.961	0.968	0.974	0.973	0.914	0.939	0.946	0.954	0.954
AEGL-2 (1/6 h)	0.928	0.934	0.940	0.944	0.943	1.000	0.993	0.986	0.968	0.963	0.965	0.965	0.959	0.940	0.939
AEGL-2 (1/2 h)	0.942	0.951	0.957	0.962	0.961	0.993	1.000	0.998	0.985	0.979	0.957	0.969	0.969	0.958	0.954
AEGL-2 (1 h)	0.945	0.955	0.961	0.968	0.968	0.986	0.998	1.000	0.993	0.986	0.949	0.968	0.971	0.965	0.961
AEGL-2 (4 h)	0.938	0.950	0.959	0.973	0.974	0.968	0.985	0.993	1.000	0.998	0.936	0.958	0.965	0.971	0.970
AEGL-2 (8 h)	0.927	0.941	0.951	0.969	0.973	0.963	0.979	0.986	0.998	1.000	0.937	0.957	0.963	0.969	0.972
AEGL-3 (1/6 h)	0.887	0.896	0.904	0.912	0.914	0.965	0.957	0.949	0.936	0.937	1.000	0.990	0.981	0.955	0.958
AEGL-3 (1/2 h)	0.914	0.923	0.930	0.938	0.939	0.965	0.969	0.968	0.958	0.957	0.990	1.000	0.997	0.982	0.981
AEGL-3 (1 h)	0.921	0.931	0.938	0.946	0.946	0.959	0.969	0.971	0.965	0.963	0.981	0.997	1.000	0.992	0.989
AEGL-3 (4 h)	0.928	0.939	0.945	0.954	0.954	0.940	0.958	0.965	0.971	0.969	0.955	0.982	0.992	1.000	0.997
AEGL-3 (8 h)	0.919	0.932	0.940	0.952	0.954	0.939	0.954	0.961	0.970	0.972	0.958	0.981	0.989	0.997	1.000

Table 3. A fifteen-by-fifteen Pearson correlation matrix of AEGLs across all five exposure duration (1/6 to 8 h) and three health severity thresholds (-1, -2, -3). Each cell represented the correlation of two duration-and-threshold-specific AEGL levels. All correlation coefficients (*r*) were at least 0.88. The highest correlations were observed for within threshold AEGL pairs (dark green cells). The lowest correlations were observed for all cross-threshold AEGL pairs at the 10 min. exposure durations (light green cells).

Duration-and-threshold-specific AEGL pairs		Model #	Coeff.	Estimate	SE	2.5% CI LL	97.5% CI UL	Reject Ho?
AEGL-1 (1/2h)	AEGL-1 (1/6 h)	1	Bo	0.04	0.01	0.02	0.06	N
			B1	0.99	0.01	0.98	1.01	Y
AEGL-1 (1 h)	AEGL-1 (1/6 h)	2	Bo	0.09	0.01	0.06	0.12	Y
			B1	0.99	0.01	0.96	1.01	Y
AEGL-1 (4 h)	AEGL-1 (1/6 h)	3	Bo	0.19	0.03	0.14	0.24	N
			B1	0.96	0.02	0.92	1.01	Y
AEGL-1 (8 h)	AEGL-1 (1/6 h)	4	Bo	0.24	0.03	0.18	0.30	N
			B1	0.95	0.03	0.90	1.00	Y
AEGL-2 (1/6 h)	AEGL-1 (1/6 h)	5	Bo	-1.27	0.07	-1.43	-1.15	N
			B1	1.08	0.03	1.02	1.15	N
AEGL-2 (1/2 h)	AEGL-1 (1/6 h)	6	Bo	-1.07	0.06	-1.19	-0.97	N
			B1	1.08	0.03	1.02	1.14	N
AEGL-2 (1 h)	AEGL-1 (1/6 h)	7	Bo	-0.89	0.05	-1.00	-0.79	N
			B1	1.06	0.03	1.01	1.12	N
AEGL-2 (4 h)	AEGL-1 (1/6 h)	8	Bo	-0.56	0.05	-0.66	-0.46	N
			B1	1.02	0.03	0.97	1.08	Y
AEGL-2 (8 h)	AEGL-1 (1/6 h)	9	Bo	-0.41	0.05	-0.52	-0.31	N
			B1	1.00	0.03	0.95	1.06	Y
AEGL-3 (1/6 h)	AEGL-1 (1/6 h)	10	Bo	-2.20	0.13	-2.49	-1.98	N
			B1	1.16	0.05	1.07	1.27	N
AEGL-3 (1/2 h)	AEGL-1 (1/6 h)	11	Bo	-1.94	0.10	-2.15	-1.78	N
			B1	1.16	0.04	1.09	1.24	N
AEGL-3 (1 h)	AEGL-1 (1/6 h)	12	Bo	-1.71	0.08	-1.89	-1.57	N
			B1	1.15	0.04	1.09	1.23	N
AEGL-3 (4 h)	AEGL-1 (1/6 h)	13	Bo	-1.23	0.06	-1.35	-1.11	N
			B1	1.09	0.03	1.04	1.15	N
AEGL-3 (8 h)	AEGL-1 (1/6 h)	14	Bo	-1.04	0.06	-1.18	-0.92	N
			B1	1.08	0.03	1.02	1.14	N
AEGL-1 (1 h)	AEGL-1 (1/2h)	15	Bo	0.05	0.01	0.03	0.06	N
			B1	0.99	0.01	0.98	1.00	Y
AEGL-1 (4 h)	AEGL-1 (1/2h)	16	Bo	0.14	0.02	0.11	0.18	N
			B1	0.97	0.01	0.94	1.00	Y
AEGL-1 (8 h)	AEGL-1 (1/2h)	17	Bo	0.20	0.03	0.15	0.25	N
			B1	0.95	0.02	0.92	0.99	N
AEGL-2 (1/6 h)	AEGL-1 (1/2h)	18	Bo	-1.32	0.06	-1.45	-1.21	N
			B1	1.09	0.03	1.03	1.15	N
AEGL-2 (1/2 h)	AEGL-1 (1/2h)	19	Bo	-1.12	0.06	-1.24	-1.01	N
			B1	1.08	0.03	1.03	1.14	N
AEGL-2 (1 h)	AEGL-1 (1/2h)	20	Bo	-0.93	0.05	-1.03	-0.84	N
			B1	1.07	0.02	1.02	1.12	N
AEGL-2 (4 h)	AEGL-1 (1/2h)	21	Bo	-0.60	0.05	-0.69	-0.51	N
			B1	1.03	0.02	0.98	1.07	Y
AEGL-2 (8 h)	AEGL-1 (1/2h)	22	Bo	-0.46	0.05	-0.56	-0.37	N
			B1	1.01	0.02	0.96	1.06	Y
AEGL-3 (1/6 h)	AEGL-1 (1/2h)	23	Bo	-2.25	0.12	-2.49	-2.04	N
			B1	1.16	0.04	1.10	1.25	N
AEGL-3 (1/2 h)	AEGL-1 (1/2h)	24	Bo	-1.99	0.10	-2.21	-1.82	N
			B1	1.16	0.04	1.10	1.25	N
AEGL-3 (1 h)	AEGL-1 (1/2h)	25	Bo	-1.76	0.08	-1.94	-1.62	N
			B1	1.15	0.03	1.09	1.22	N
AEGL-3 (4 h)	AEGL-1 (1/2h)	26	Bo	-1.27	0.06	-1.40	-1.17	N
			B1	1.10	0.03	1.05	1.15	N
AEGL-3 (8 h)	AEGL-1 (1/2h)	27	Bo	-1.09	0.06	-1.21	-0.98	N
			B1	1.08	0.03	1.03	1.13	N
AEGL-1 (4 h)	AEGL-1 (1 h)	28	Bo	0.10	0.01	0.07	0.12	N
			B1	0.98	0.01	0.96	0.99	N
AEGL-1 (8 h)	AEGL-1 (1 h)	29	Bo	0.15	0.02	0.12	0.19	N
			B1	0.96	0.01	0.93	0.99	N
AEGL-2 (1/6 h)	AEGL-1 (1 h)	30	Bo	-1.38	0.06	-1.51	-1.26	N
			B1	1.09	0.03	1.04	1.15	N
AEGL-2 (1/2 h)	AEGL-1 (1 h)	31	Bo	-1.18	0.05	-1.29	-1.08	N
			B1	1.09	0.03	1.04	1.14	N
AEGL-2 (1 h)	AEGL-1 (1 h)	32	Bo	-0.99	0.05	-1.09	-0.90	N
			B1	1.08	0.02	1.03	1.12	N
AEGL-2 (4 h)	AEGL-1 (1 h)	34	Bo	-0.65	0.04	-0.73	-0.58	N
			B1	1.03	0.02	0.99	1.08	Y
AEGL-2 (8 h)	AEGL-1 (1 h)	35	Bo	-0.51	0.04	-0.60	-0.43	N
			B1	1.01	0.02	0.97	1.06	Y
AEGL-3 (1/6 h)	AEGL-1 (1 h)	36	Bo	-2.32	0.12	-2.59	-2.10	N
			B1	1.18	0.05	1.09	1.27	N
AEGL-3 (1/2 h)	AEGL-1 (1 h)	37	Bo	-2.06	0.09	-2.26	-1.89	N
			B1	1.17	0.04	1.11	1.25	N
AEGL-3 (1 h)	AEGL-1 (1 h)	38	Bo	-1.82	0.08	-1.99	-1.69	N
			B1	1.16	0.03	1.10	1.23	N
AEGL-3 (4 h)	AEGL-1 (1 h)	39	Bo	-1.33	0.06	-1.44	-1.23	N
			B1	1.11	0.02	1.06	1.15	N
AEGL-3 (8 h)	AEGL-1 (1 h)	39	Bo	-1.15	0.06	-1.26	-1.04	N
			B1	1.09	0.02	1.04	1.14	N
AEGL-1 (8 h)	AEGL-1 (4 h)	40	Bo	0.06	0.01	0.04	0.07	N
			B1	0.99	0.01	0.98	1.00	Y
AEGL-2 (1/6 h)	AEGL-1 (4 h)	41	Bo	-1.52	0.07	-1.67	-1.38	N
			B1	1.12	0.04	1.05	1.19	N
AEGL-2 (1/2 h)	AEGL-1 (4 h)	42	Bo	-1.32	0.06	-1.45	-1.21	N
			B1	1.11	0.03	1.06	1.18	N
AEGL-2 (1 h)	AEGL-1 (4 h)	43	Bo	-1.12	0.05	-1.22	-1.03	N
			B1	1.10	0.03	1.05	1.15	N
AEGL-2 (4 h)	AEGL-1 (4 h)	44	Bo	-0.79	0.04	-0.86	-0.71	N
			B1	1.06	0.02	1.02	1.10	N
AEGL-2 (8 h)	AEGL-1 (4 h)	45	Bo	-0.64	0.04	-0.72	-0.57	N
			B1	1.04	0.02	1.00	1.08	Y
AEGL-3 (1/6 h)	AEGL-1 (4 h)	46	Bo	-2.48	0.12	-2.75	-2.27	N
			B1	1.21	0.05	1.12	1.31	N
AEGL-3 (1/2 h)	AEGL-1 (4 h)	47	Bo	-2.22	0.10	-2.44	-2.04	N
			B1	1.20	0.04	1.13	1.29	N
AEGL-3 (1 h)	AEGL-1 (4 h)	48	Bo	-1.98	0.09	-2.16	-1.83	N
			B1	1.19	0.03	1.13	1.27	N
AEGL-3 (4 h)	AEGL-1 (4 h)	49	Bo	-1.48	0.06	-1.61	-1.36	N
			B1	1.14	0.03	1.09	1.19	N
AEGL-3 (8 h)	AEGL-1 (4 h)	50	Bo	-1.29	0.06	-1.41	-1.18	N
			B1	1.12	0.02	1.07	1.17	N

Table 4. Deming linear regression estimates for each of the 105 unique duration-and-threshold specific AEGL pairs. Estimates include the slope (B1), intercept (Bo), and their standard errors (SE) and 95% confidence intervals (CIs). Hypothesis testing of database comparability showed statistical identity of Deming slopes and y-intercepts (Reject Ho?: N=no, Y=yes). Cells highlighted with purple font have statistically identical slopes (95% CI_{B1} includes 1), and cells highlighted with green font have statistically identical intercepts (95% CI_{Bo} includes 0).

Table 4 (1 of 2)

Duration-and-threshold-specific AEGL pairs		Model #	Coeff.	Estimate	SE	2.5% CI LL	97.5% CI UL	Reject Ho?
AEGL-2 (1/6 h)	AEGL-1 (8 h)	51	Bo	-1.60	0.08	-1.77	-1.46	N
			B1	1.14	0.04	1.07	1.22	N
AEGL-2 (1/2 h)	AEGL-1 (8 h)	52	Bo	-1.39	0.06	-1.53	-1.28	N
			B1	1.13	0.03	1.07	1.20	N
AEGL-2 (1 h)	AEGL-1 (8 h)	53	Bo	-1.20	0.05	-1.30	-1.11	N
			B1	1.12	0.03	1.06	1.17	N
AEGL-2 (4 h)	AEGL-1 (8 h)	54	Bo	-0.86	0.04	-0.94	-0.78	N
			B1	1.07	0.02	1.03	1.12	N
AEGL-2 (8 h)	AEGL-1 (8 h)	55	Bo	-0.71	0.04	-0.79	-0.64	N
			B1	1.05	0.02	1.02	1.10	N
AEGL-3 (1/6 h)	AEGL-1 (8 h)	56	Bo	-2.59	0.12	-2.83	-2.37	N
			B1	1.23	0.05	1.14	1.33	N
AEGL-3 (1/2 h)	AEGL-1 (8 h)	57	Bo	-2.32	0.10	-2.54	-2.14	N
			B1	1.23	0.04	1.15	1.32	N
AEGL-3 (1 h)	AEGL-1 (8 h)	58	Bo	-2.07	0.09	-2.26	-1.89	N
			B1	1.22	0.04	1.15	1.29	N
AEGL-3 (4 h)	AEGL-1 (8 h)	59	Bo	-1.56	0.06	-1.68	-1.44	N
			B1	1.16	0.03	1.10	1.21	N
AEGL-3 (8 h)	AEGL-1 (8 h)	60	Bo	-1.37	0.06	-1.49	-1.26	N
			B1	1.14	0.03	1.09	1.20	N
AEGL-2 (1/2 h)	AEGL-2 (1/6 h)	61	Bo	0.18	0.01	0.15	0.20	N
			B1	0.99	0.01	0.98	1.01	Y
AEGL-2 (1 h)	AEGL-2 (1/6 h)	62	Bo	0.35	0.02	0.32	0.39	N
			B1	0.98	0.01	0.96	1.00	Y
AEGL-2 (4 h)	AEGL-2 (1/6 h)	63	Bo	0.69	0.02	0.64	0.73	N
			B1	0.93	0.02	0.91	0.97	N
AEGL-2 (8 h)	AEGL-2 (1/6 h)	64	Bo	0.86	0.02	0.81	0.91	N
			B1	0.90	0.02	0.87	0.93	N
AEGL-3 (1/6 h)	AEGL-2 (1/6 h)	65	Bo	-0.70	0.04	-0.78	-0.62	N
			B1	1.03	0.02	1.01	1.07	N
AEGL-3 (1/2 h)	AEGL-2 (1/6 h)	66	Bo	-0.49	0.04	-0.56	-0.42	N
			B1	1.03	0.02	1.00	1.06	Y
AEGL-3 (1 h)	AEGL-2 (1/6 h)	67	Bo	-0.29	0.04	-0.37	-0.23	N
			B1	1.02	0.02	0.99	1.06	Y
AEGL-3 (4 h)	AEGL-2 (1/6 h)	68	Bo	0.13	0.04	0.06	0.20	N
			B1	0.98	0.02	0.95	1.02	Y
AEGL-3 (8 h)	AEGL-2 (1/6 h)	69	Bo	0.34	0.03	0.27	0.41	N
			B1	0.95	0.02	0.91	1.00	Y
AEGL-2 (1 h)	AEGL-2 (1/2 h)	70	Bo	0.18	0.01	0.16	0.19	N
			B1	0.99	0.00	0.98	0.99	N
AEGL-2 (4 h)	AEGL-2 (1/2 h)	71	Bo	0.52	0.02	0.48	0.55	N
			B1	0.94	0.01	0.92	0.96	N
AEGL-2 (8 h)	AEGL-2 (1/2 h)	72	Bo	0.69	0.02	0.65	0.72	N
			B1	0.91	0.01	0.88	0.93	N
AEGL-3 (1/6 h)	AEGL-2 (1/2 h)	73	Bo	-0.89	0.05	-0.97	-0.80	N
			B1	1.04	0.02	1.00	1.08	Y
AEGL-3 (1/2 h)	AEGL-2 (1/2 h)	74	Bo	-0.68	0.04	-0.75	-0.61	N
			B1	1.04	0.02	1.00	1.07	Y
AEGL-3 (1 h)	AEGL-2 (1/2 h)	75	Bo	-0.48	0.03	-0.54	-0.42	N
			B1	1.03	0.02	1.00	1.06	Y
AEGL-3 (4 h)	AEGL-2 (1/2 h)	76	Bo	-0.05	0.03	-0.12	0.02	Y
			B1	0.98	0.02	0.95	1.02	Y
AEGL-3 (8 h)	AEGL-2 (1/2 h)	77	Bo	0.16	0.03	0.10	0.23	N
			B1	0.95	0.02	0.92	0.99	N
AEGL-2 (8 h)	AEGL-2 (1 h)	79	Bo	0.52	0.02	0.49	0.55	N
			B1	0.92	0.01	0.90	0.93	N
AEGL-3 (1/6 h)	AEGL-2 (1 h)	80	Bo	-1.07	0.05	-1.18	-0.98	N
			B1	1.05	0.02	1.01	1.09	N
AEGL-3 (1/2 h)	AEGL-2 (1 h)	81	Bo	-0.86	0.04	-0.94	-0.79	N
			B1	1.05	0.02	1.02	1.08	N
AEGL-3 (1 h)	AEGL-2 (1 h)	82	Bo	-0.66	0.03	-0.73	-0.60	N
			B1	1.04	0.02	1.01	1.07	N
AEGL-3 (4 h)	AEGL-2 (1 h)	83	Bo	-0.23	0.03	-0.29	-0.16	N
			B1	0.99	0.02	0.96	1.03	Y
AEGL-3 (8 h)	AEGL-2 (1 h)	84	Bo	-0.01	0.03	-0.07	0.05	Y
			B1	0.96	0.02	0.93	1.00	Y
AEGL-2 (8 h)	AEGL-2 (1 h)	85	Bo	0.18	0.01	0.17	0.20	N
			B1	0.96	0.00	0.96	0.97	N
AEGL-3 (1/6 h)	AEGL-2 (4 h)	86	Bo	-1.48	0.06	-1.61	-1.37	N
			B1	1.10	0.03	1.05	1.16	N
AEGL-3 (1/2 h)	AEGL-2 (4 h)	87	Bo	-1.27	0.05	-1.36	-1.18	N
			B1	1.10	0.02	1.06	1.14	N
AEGL-3 (1 h)	AEGL-2 (4 h)	88	Bo	-1.06	0.04	-1.14	-0.99	N
			B1	1.09	0.02	1.05	1.13	N
AEGL-3 (4 h)	AEGL-2 (4 h)	89	Bo	-0.60	0.03	-0.66	-0.55	N
			B1	1.04	0.02	1.01	1.08	N
AEGL-3 (8 h)	AEGL-2 (4 h)	90	Bo	-0.38	0.03	-0.44	-0.32	N
			B1	1.01	0.02	0.98	1.04	Y
AEGL-3 (1/6 h)	AEGL-2 (8 h)	91	Bo	-1.73	0.07	-1.86	-1.61	N
			B1	1.14	0.03	1.09	1.21	N
AEGL-3 (1/2 h)	AEGL-2 (8 h)	92	Bo	-1.51	0.05	-1.61	-1.41	N
			B1	1.14	0.02	1.10	1.19	N
AEGL-3 (1 h)	AEGL-2 (8 h)	93	Bo	-1.29	0.04	-1.38	-1.22	N
			B1	1.13	0.02	1.09	1.17	N
AEGL-3 (4 h)	AEGL-2 (8 h)	94	Bo	-0.81	0.03	-0.88	-0.75	N
			B1	1.08	0.02	1.05	1.12	N
AEGL-3 (8 h)	AEGL-2 (8 h)	95	Bo	-0.58	0.03	-0.64	-0.53	N
			B1	1.05	0.02	1.02	1.08	N
AEGL-3 (1/2 h)	AEGL-3 (1/6 h)	96	Bo	0.20	0.02	0.16	0.23	N
			B1	1.00	0.01	0.98	1.02	Y
AEGL-3 (1 h)	AEGL-3 (1/6 h)	97	Bo	0.39	0.02	0.35	0.43	N
			B1	0.99	0.01	0.96	1.01	Y
AEGL-3 (4 h)	AEGL-3 (1/6 h)	98	Bo	0.79	0.03	0.73	0.85	N
			B1	0.95	0.02	0.92	0.99	N
AEGL-3 (8 h)	AEGL-3 (1/6 h)	99	Bo	0.99	0.03	0.94	1.05	N
			B1	0.92	0.02	0.89	0.96	N
AEGL-3 (1 h)	AEGL-3 (1/2 h)	100	Bo	0.19	0.01	0.18	0.21	N
			B1	0.99	0.00	0.98	1.00	Y
AEGL-3 (4 h)	AEGL-3 (1/2 h)	101	Bo	0.60	0.02	0.56	0.64	N
			B1	0.95	0.01	0.93	0.98	N
AEGL-3 (8 h)	AEGL-3 (1/2 h)	102	Bo	0.80	0.02	0.77	0.84	N
			B1	0.92	0.01	0.90	0.95	N
AEGL-3 (4 h)	AEGL-3 (1 h)	103	Bo	0.41	0.01	0.39	0.44	N
			B1	0.96	0.01	0.95	0.98	N
AEGL-3 (8 h)	AEGL-3 (1 h)	104	Bo	0.62	0.02	0.59	0.65	N
			B1	0.93	0.01	0.91	0.95	N
AEGL-3 (8 h)	AEGL-3 (4 h)	105	Bo	0.21	0.01	0.20	0.23	N
			B1	0.97	0.00	0.96	0.98	N

Table 4 (2 of 2)

	AEGL-1 (1/6 h)	AEGL-1 (1/2 h)	AEGL-1 (1 h)	AEGL-1 (4 h)	AEGL-1 (8 h)	AEGL-2 (1/6 h)	AEGL-2 (1/2 h)	AEGL-2 (1 h)	AEGL-2 (4 h)	AEGL-2 (8 h)	AEGL-3 (1/6 h)	AEGL-3 (1/2 h)	AEGL-3 (1 h)	AEGL-3 (4 h)	AEGL-3 (8 h)
AEGL-1 (1/6 h)			a_o												
AEGL-1 (1/2 h)															
AEGL-1 (1 h)															
AEGL-1 (4 h)															
AEGL-1 (8 h)															
AEGL-2 (1/6 h)															
AEGL-2 (1/2 h)													a_o		
AEGL-2 (1 h)															a_o
AEGL-2 (4 h)															
AEGL-2 (8 h)															
AEGL-3 (1/6 h)															
AEGL-3 (1/2 h)															
AEGL-3 (1 h)															
AEGL-3 (4 h)															
AEGL-3 (8 h)															

Table 5. Distribution of duration-and-threshold-specific AEGL pairs with observed statistical identity. Cells highlighted in purple indicate AEGL pairs with statistically identical slopes and cells with 'a_o' indicate AEGL pairs with statistically identical intercepts.

	AEGL-1 (1/6 h)	AEGL-1 (1/2 h)	AEGL-1 (1 h)	AEGL-1 (4 h)	AEGL-1 (8 h)	AEGL-2 (1/6 h)	AEGL-2 (1/2 h)	AEGL-2 (1 h)	AEGL-2 (4 h)	AEGL-2 (8 h)	AEGL-3 (1/6 h)	AEGL-3 (1/2 h)	AEGL-3 (1 h)	AEGL-3 (4 h)	AEGL-3 (8 h)
AEGL-1 (1/6 h)		143	117	112	112	0	2	0	0	5	0	0	0	1	0
AEGL-1 (1/2 h)			117	112	112	0	0	2	0	5	0	0	0	0	0
AEGL-1 (1 h)				115	115	0	0	0	1	0	0	0	0	1	0
AEGL-1 (4 h)					123	0	0	0	0	0	0	0	0	0	0
AEGL-1 (8 h)						0	0	0	0	0	0	0	0	0	0
AEGL-2 (1/6 h)							65	23	19	19	0	3	31	3	0
AEGL-2 (1/2 h)								24	20	20	0	0	0	3	1
AEGL-2 (1 h)									23	23	0	0	0	2	3
AEGL-2 (4 h)										64	0	0	0	0	2
AEGL-2 (8 h)											0	0	0	0	0
AEGL-3 (1/6 h)												57	16	12	12
AEGL-3 (1/2 h)													17	13	13
AEGL-3 (1 h)														14	14
AEGL-3 (4 h)															57
AEGL-3 (8 h)															

Table 6. Distribution of identical surrogate values across AEGL levels of varying exposure durations and health severity thresholds. The numbers represent the frequency of compounds with identical AEGL values in their corresponding duration-and-threshold-specific AEGL level. Darker purple cells also indicate AEGL levels with a higher frequency of identical surrogates. The AEGL-1 threshold had the most compounds in which identical values were used across multiple exposure durations.

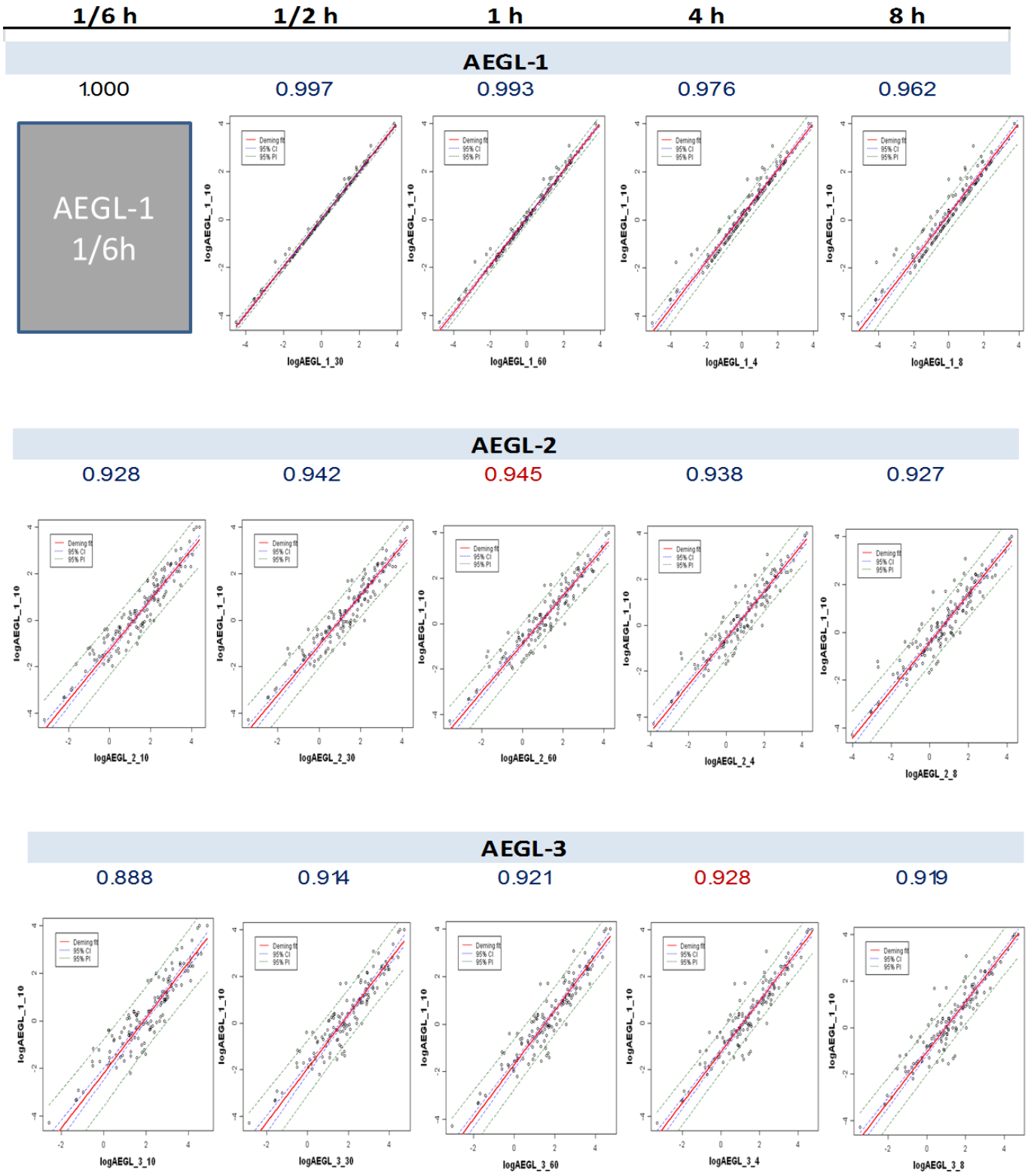


Figure 2. For each of the 15 duration-and-threshold-specific AEGL levels (y-axis), 14 cross-threshold and/or cross-exposure-duration univariate DLR models were constructed. Their respective slope (red), 95% CIs (blue) and 95% PIs (green) of the regression line, and correlation coefficients are presented. The highest correlations for cross-threshold models are in red font. Assessment of the 95% PI width and correlation coefficient for all models showed similar trends: DLR models with narrower 95% PIs generally had higher correlations.

Figure 2 (1 of 15)

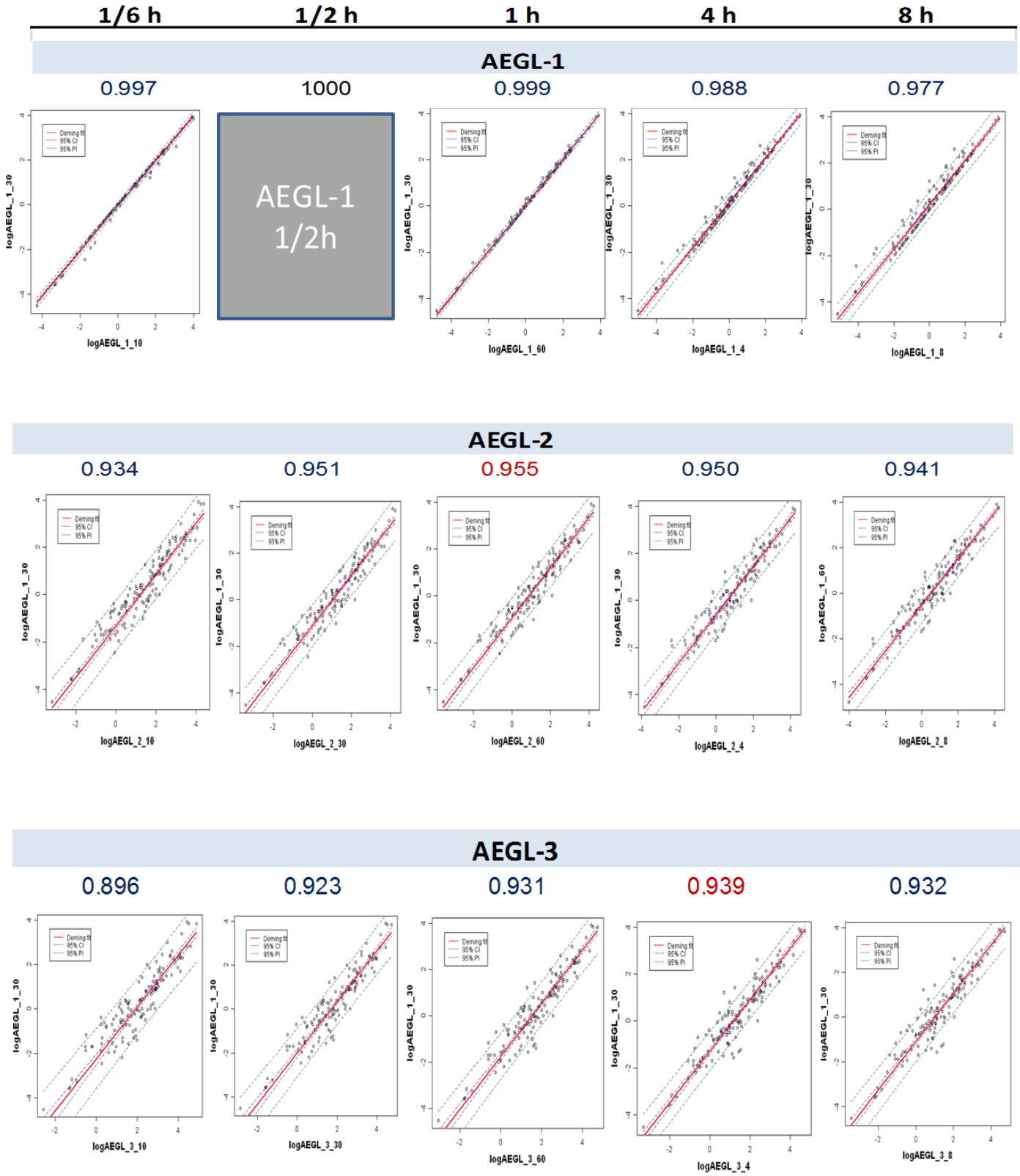


Figure 2 (2 of 15)

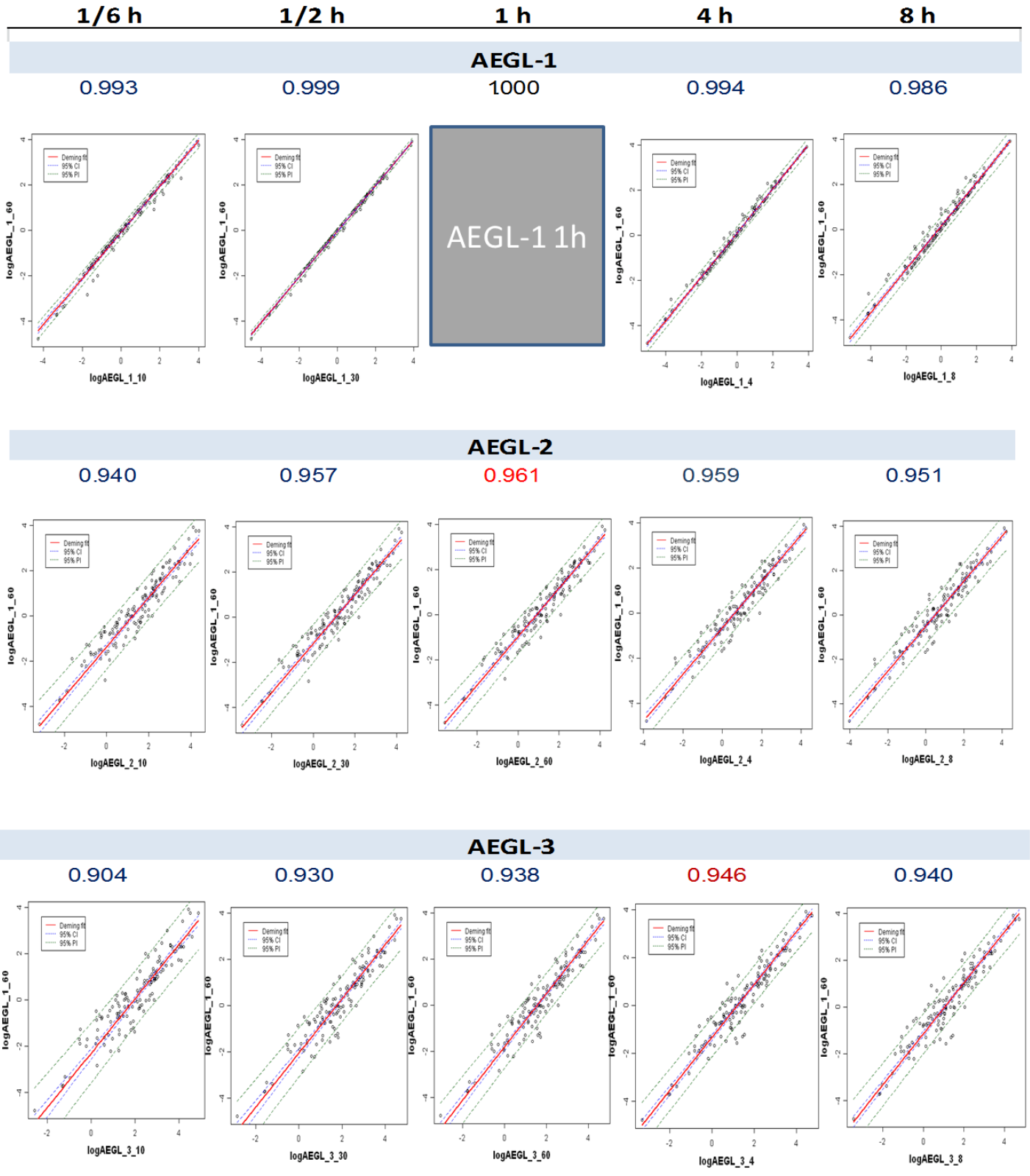
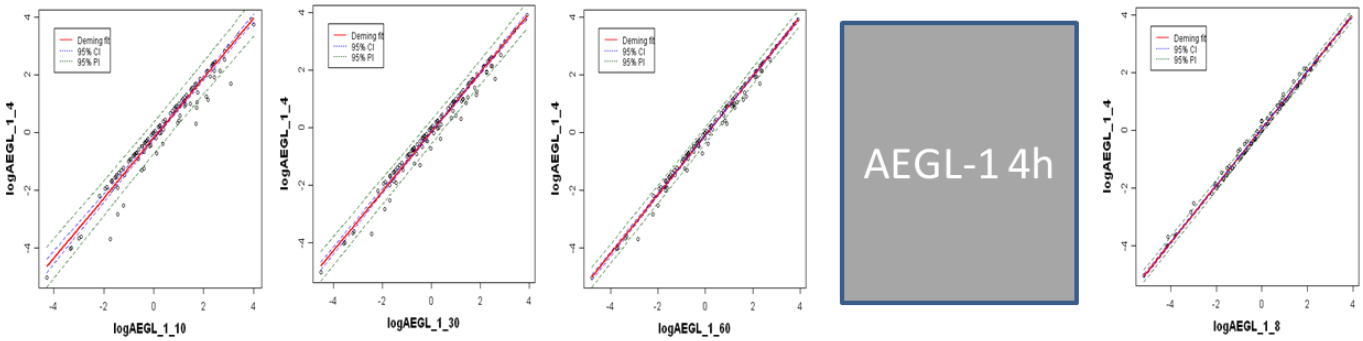
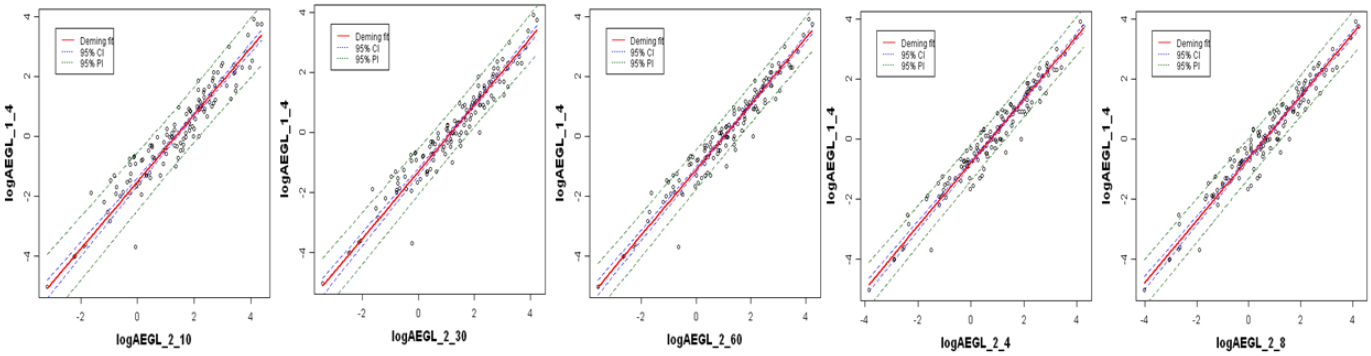


Figure 2 (3 of 15)

1/6 h	1/2 h	1 h	4 h	8 h
AEGL-1				
1.000	0.997	0.993	0.976	0.962



AEGL-2				
0.944	0.962	0.968	0.973	0.969



AEGL-3				
0.913	0.938	0.946	0.954	0.952

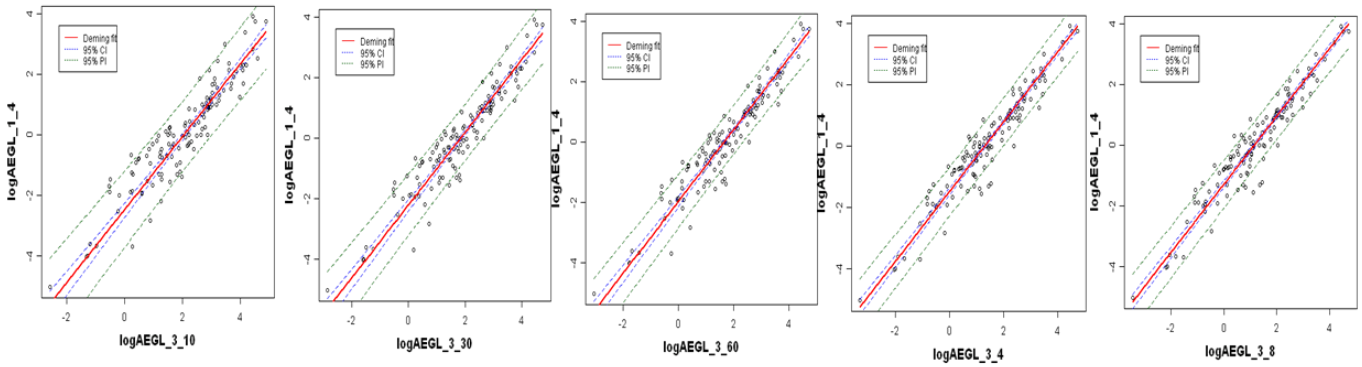
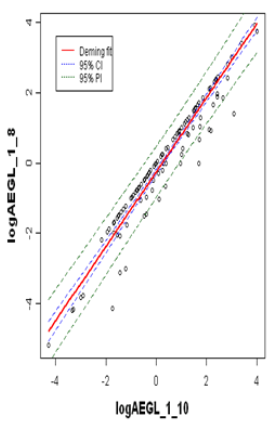
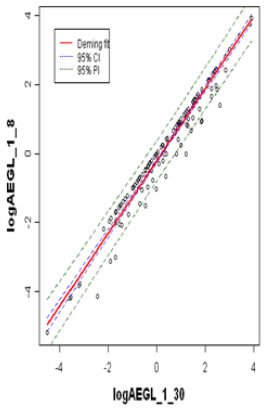
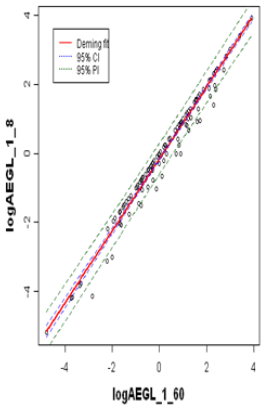


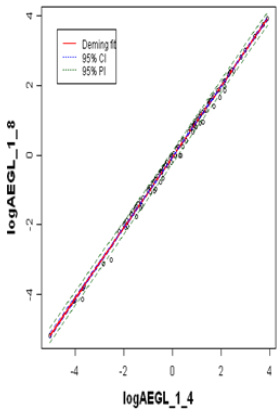
Figure 2 (4 of 15)

1/6 h	1/2 h	1 h	4 h	8 h
AEGL-1				
0.962	0.977	0.986	0.998	1.000

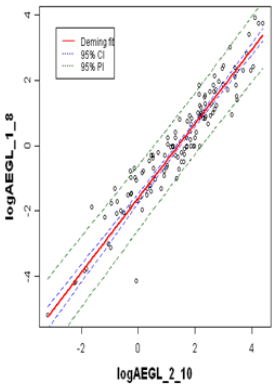


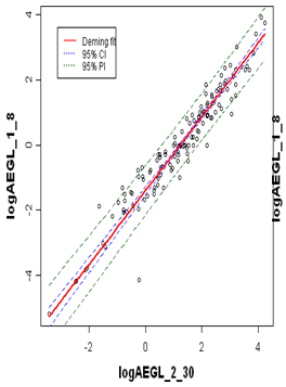


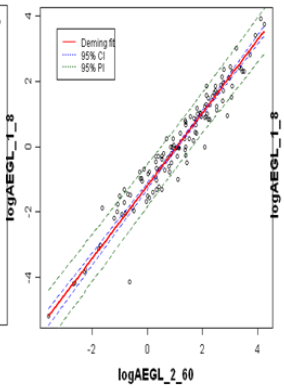


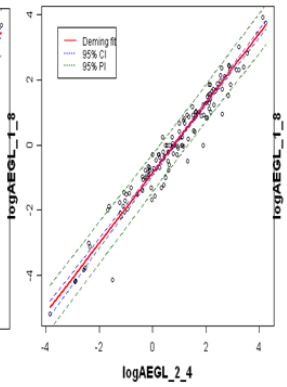


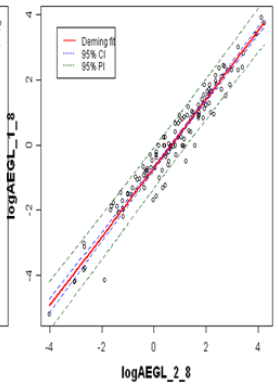
AEGL-2				
0.943	0.961	0.968	0.974	0.973



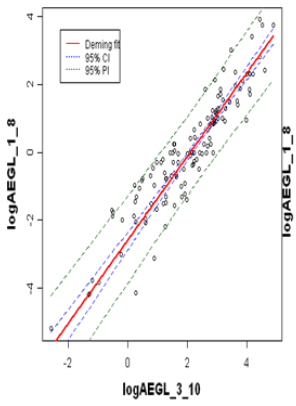


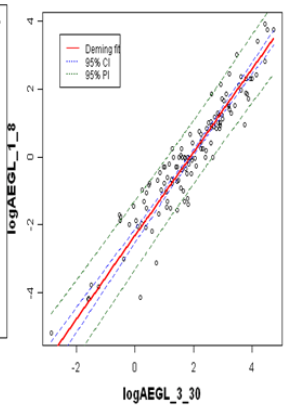


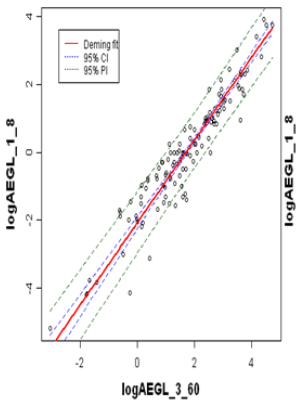


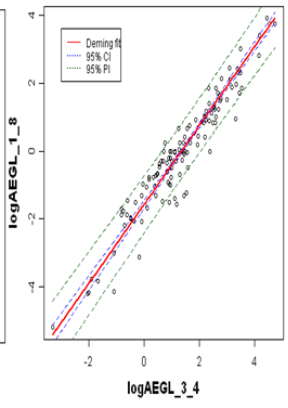


AEGL-3				
0.914	0.939	0.946	0.954	0.954









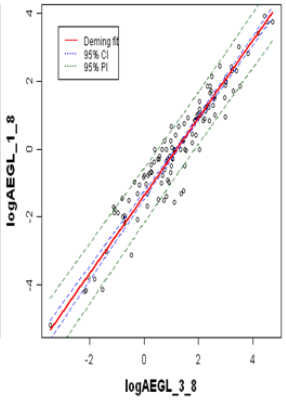


Figure 2 (5 of 15)

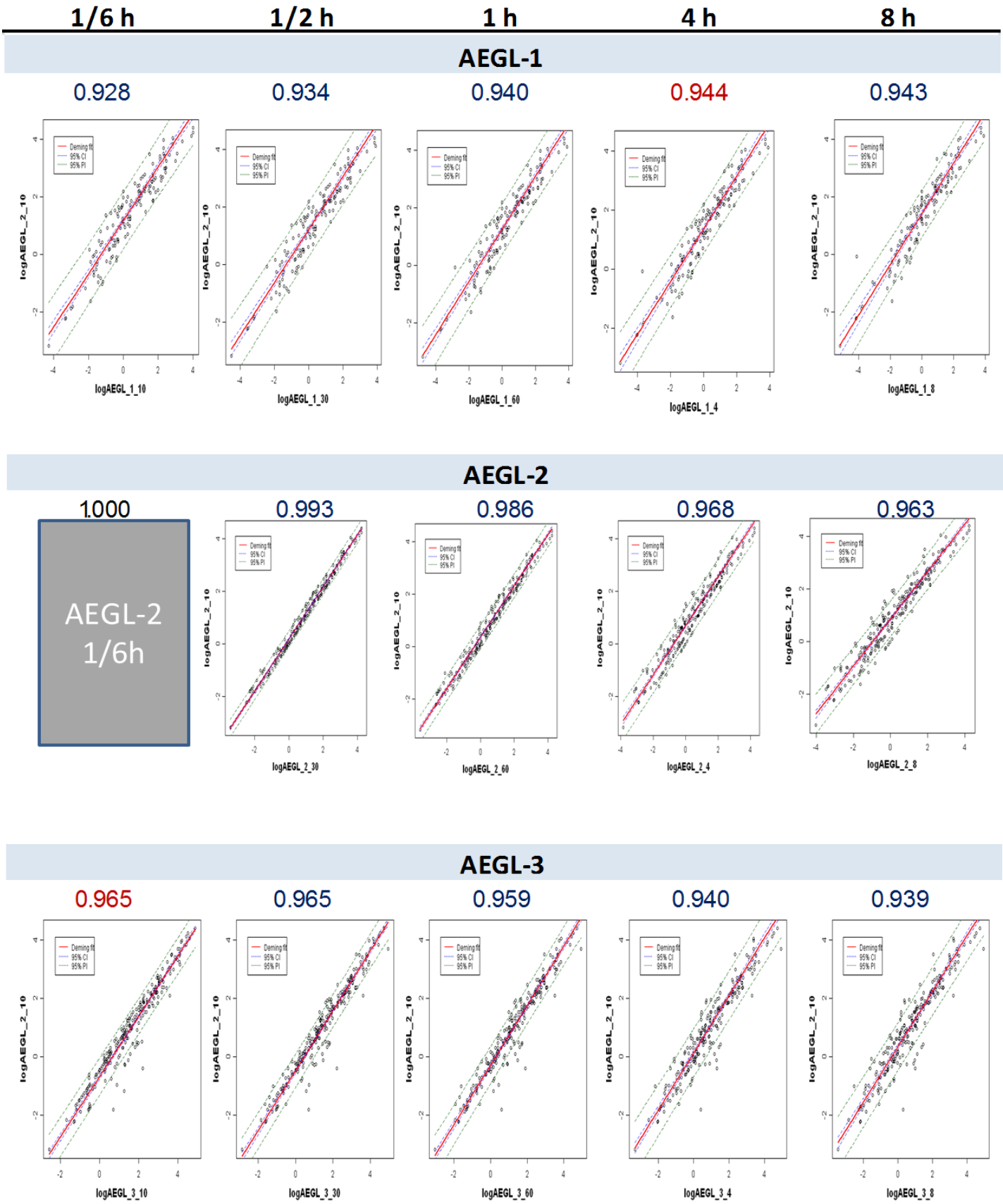


Figure 2 (6 of 15)

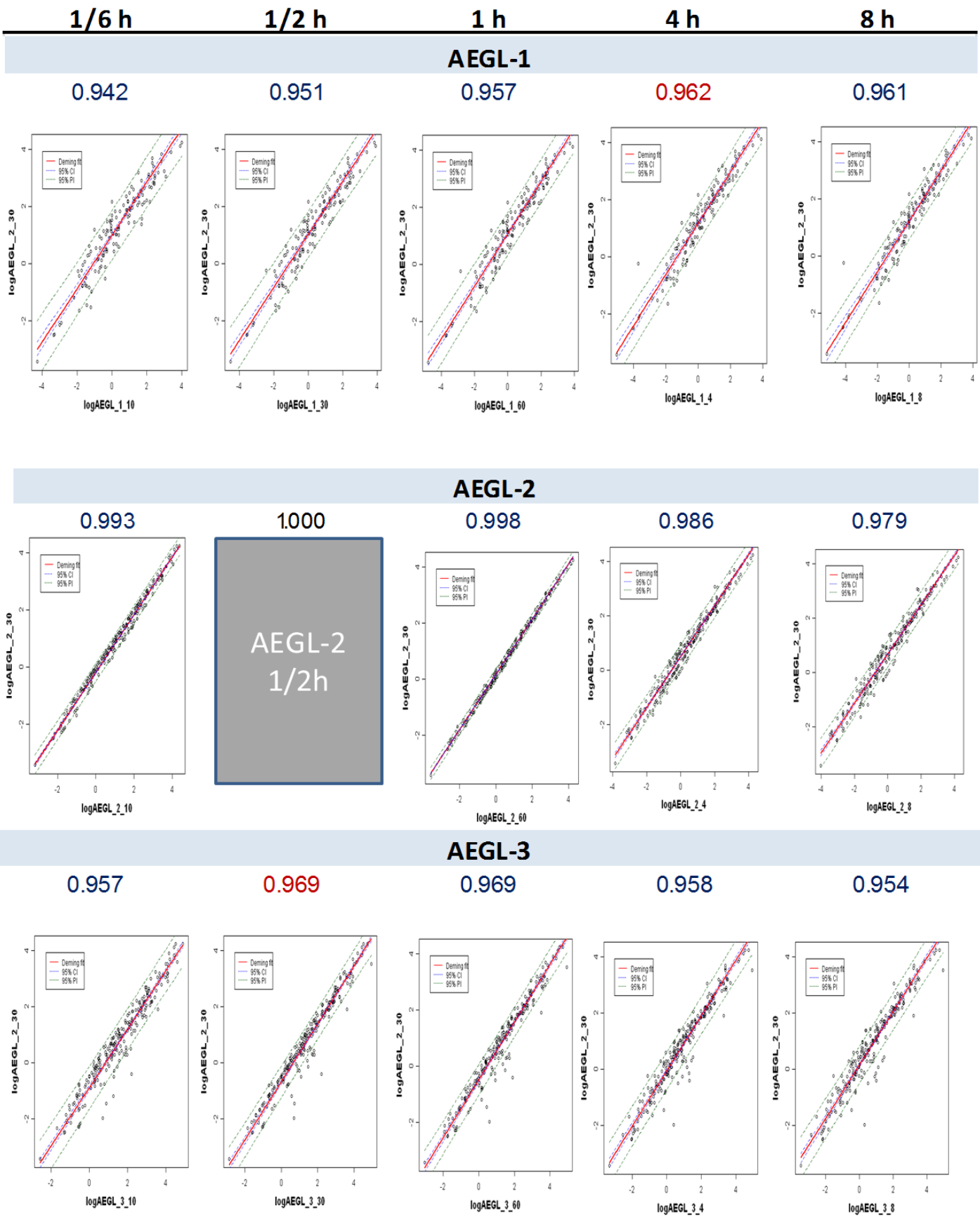


Figure 2 (7 of 15)

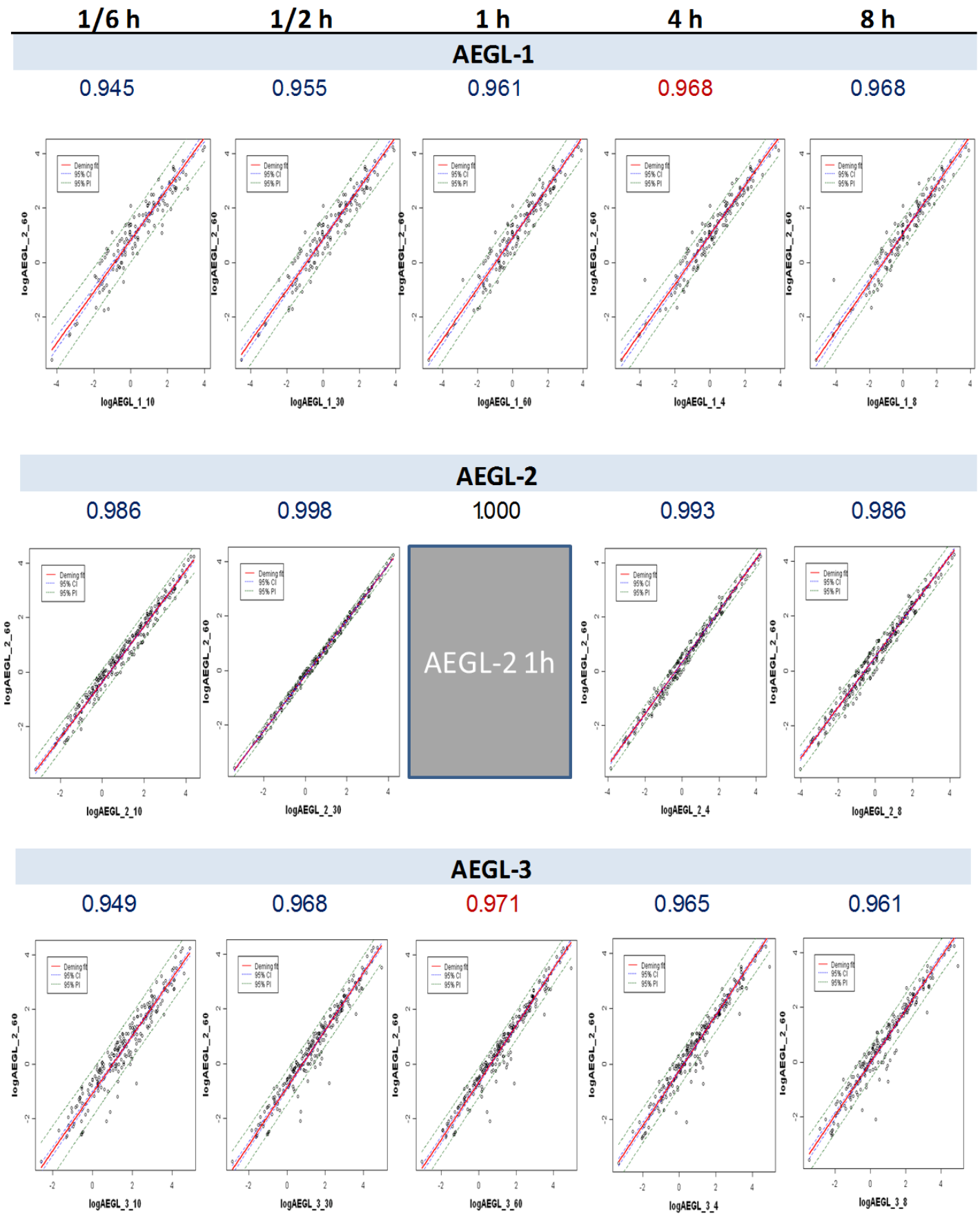


Figure 2 (8 of 15)

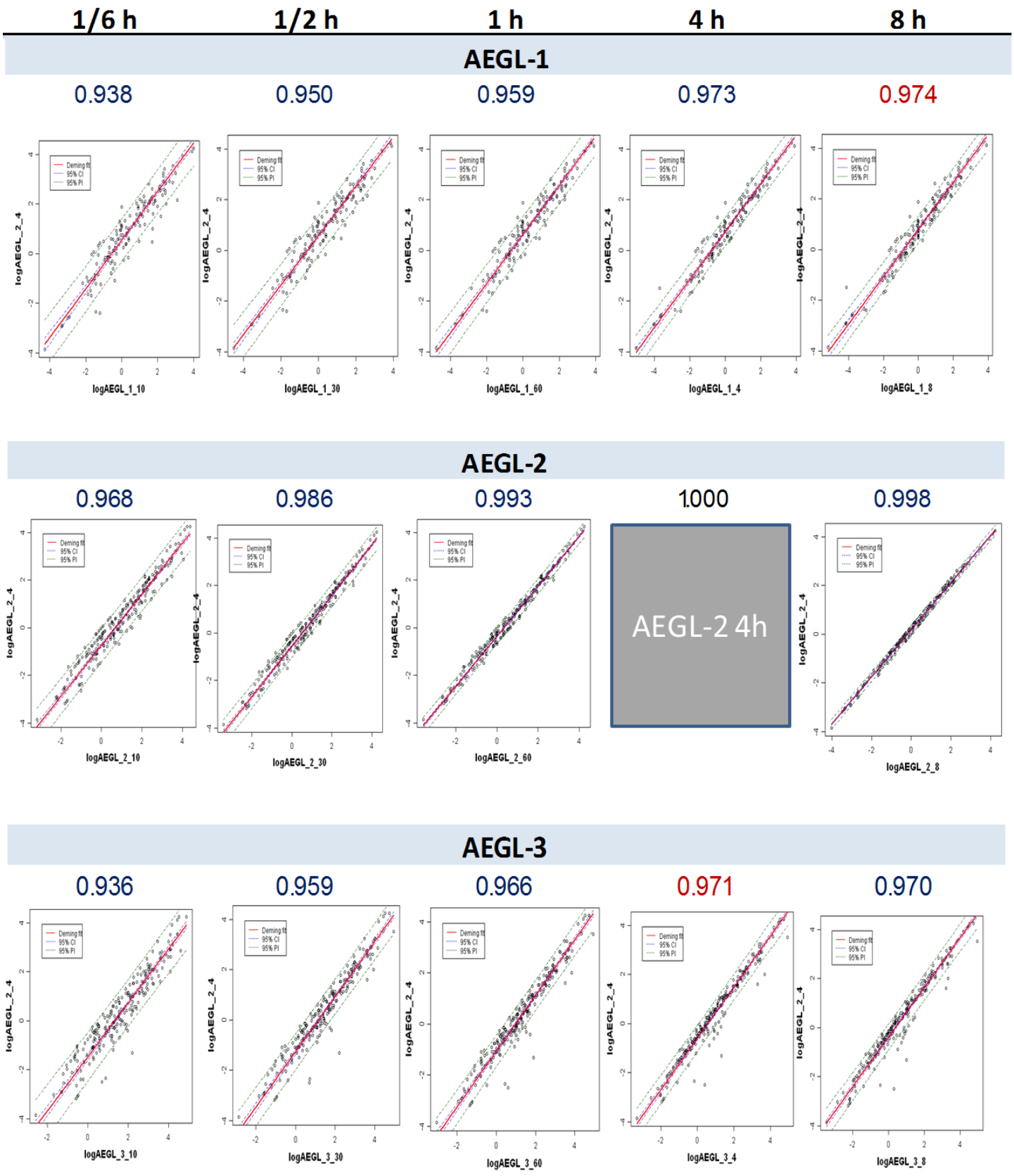


Figure 2 (9 of 15)

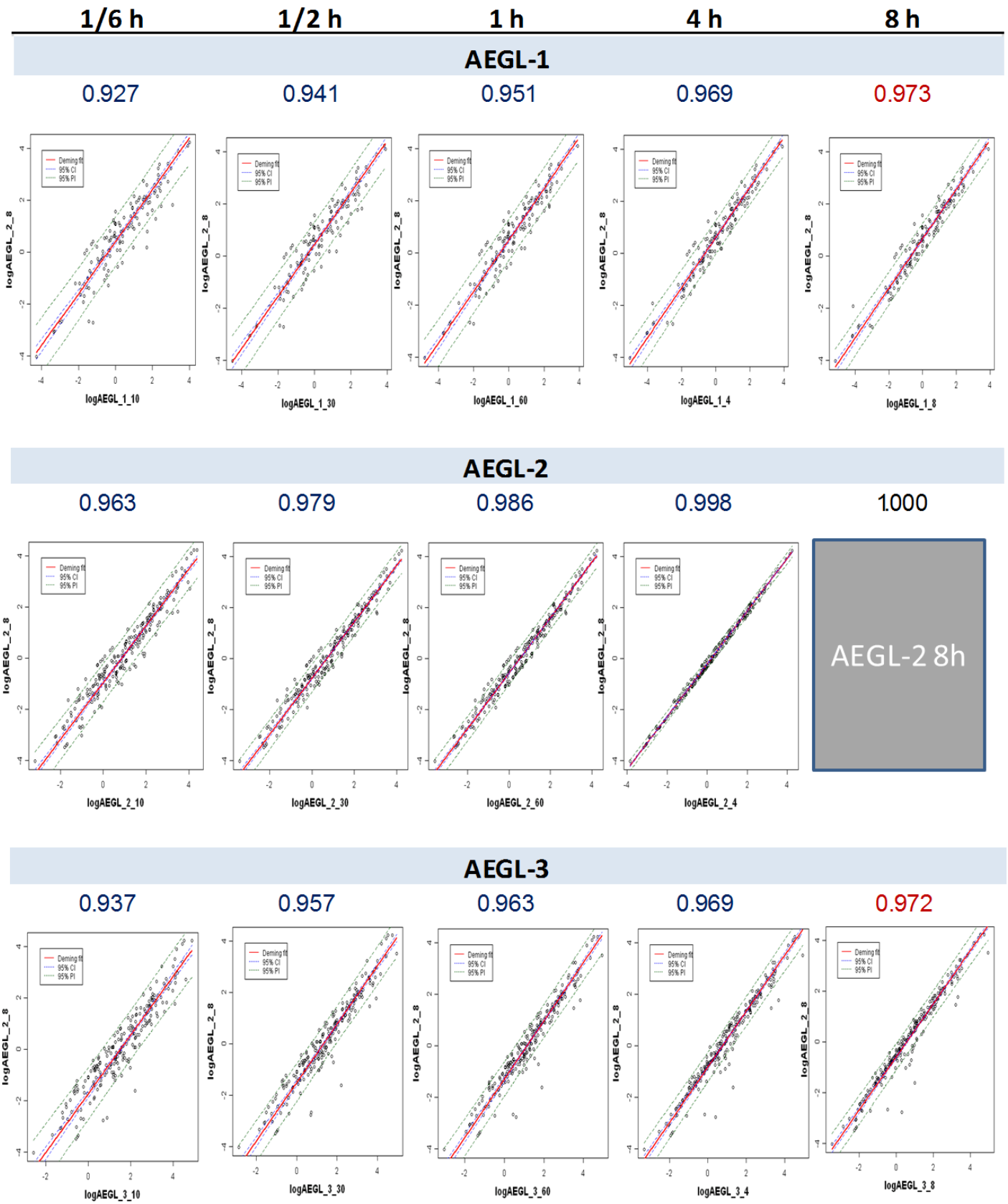


Figure 2 (10 of 15)

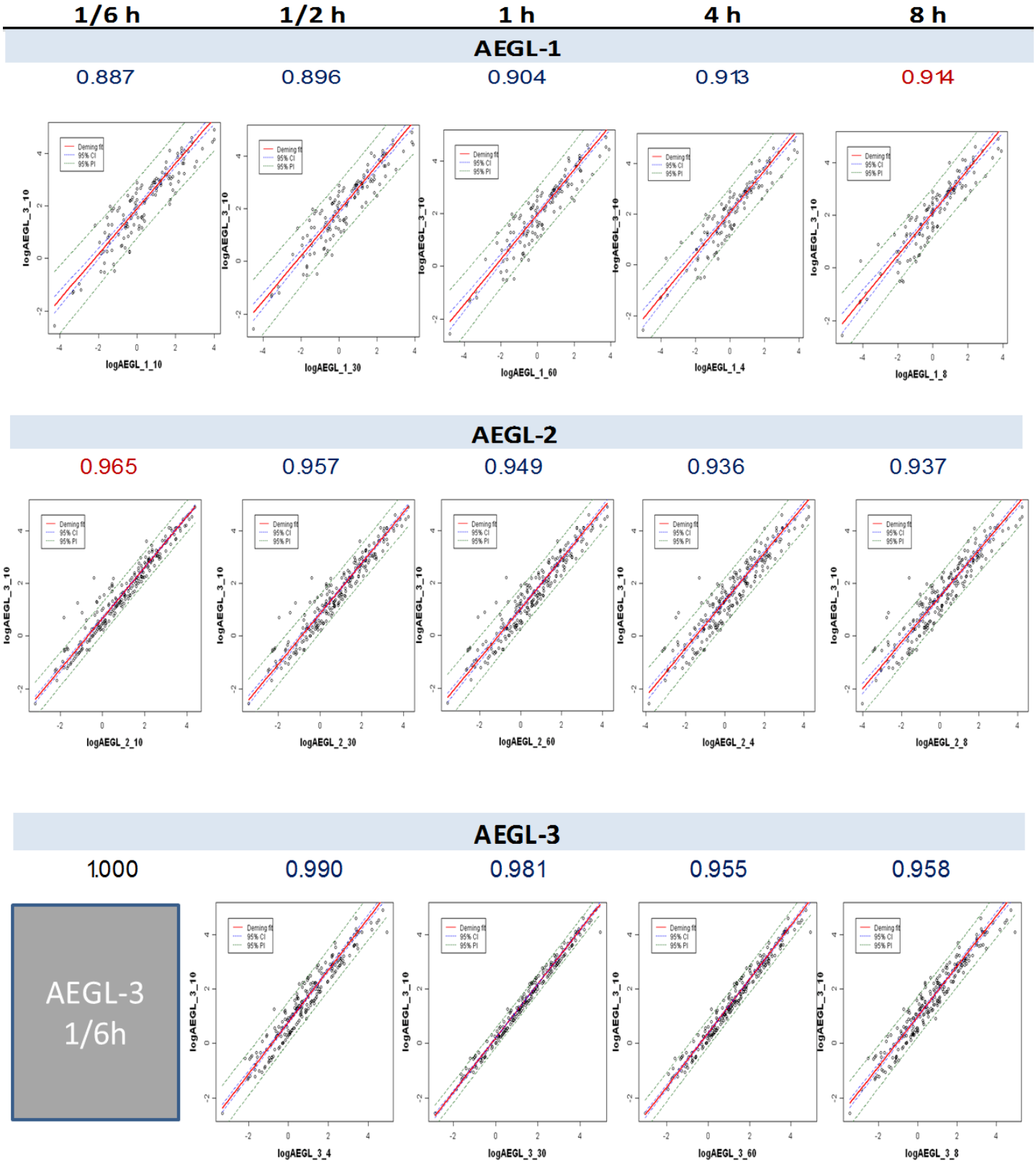
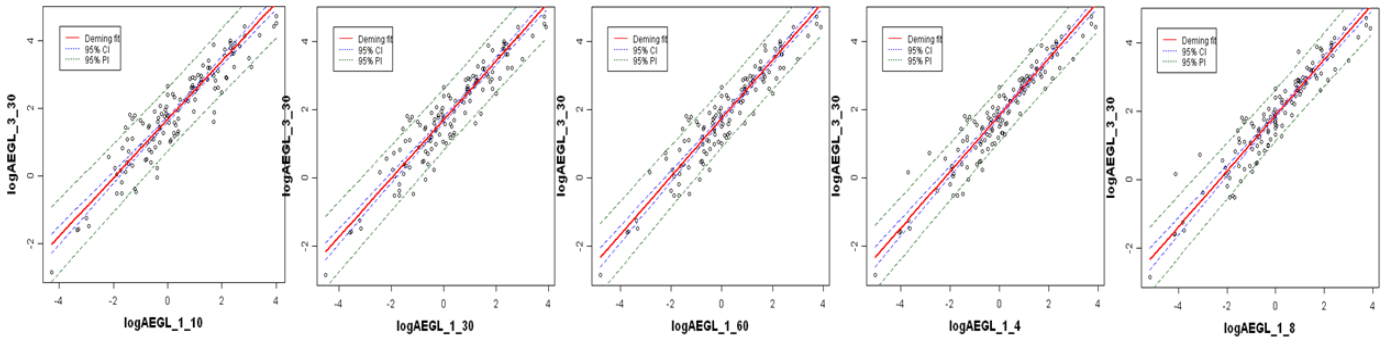
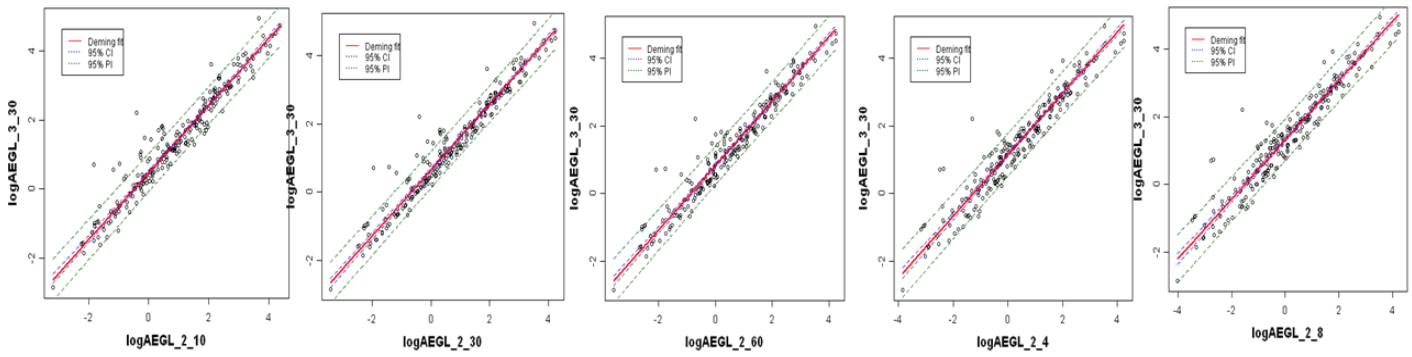


Figure 2 (11 of 15)

1/6 h	1/2 h	1 h	4 h	8 h
AEGL-1				
0.914	0.923	0.930	0.938	0.939



AEGL-2				
0.965	0.969	0.968	0.959	0.957



AEGL-3				
0.990	1.000	0.997	0.982	0.981

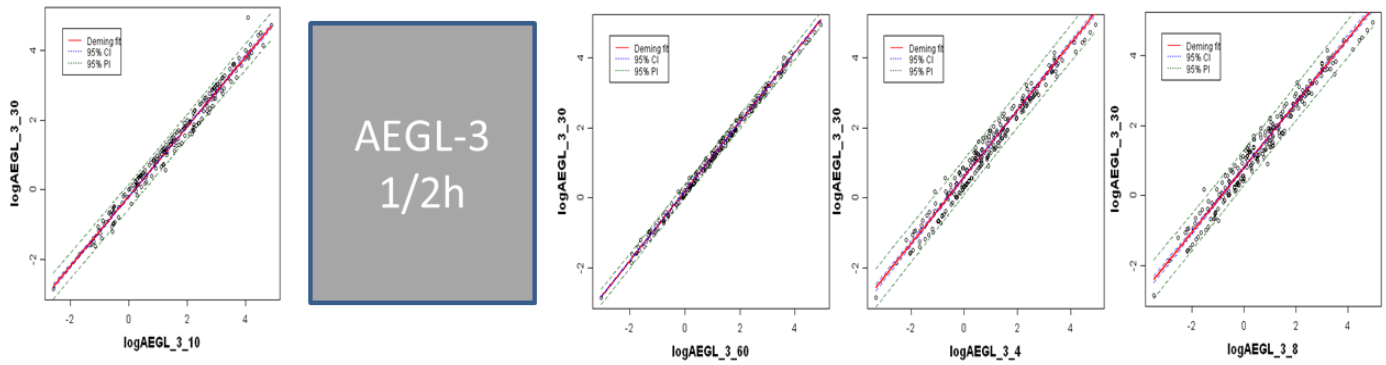


Figure 2 (12 of 15)

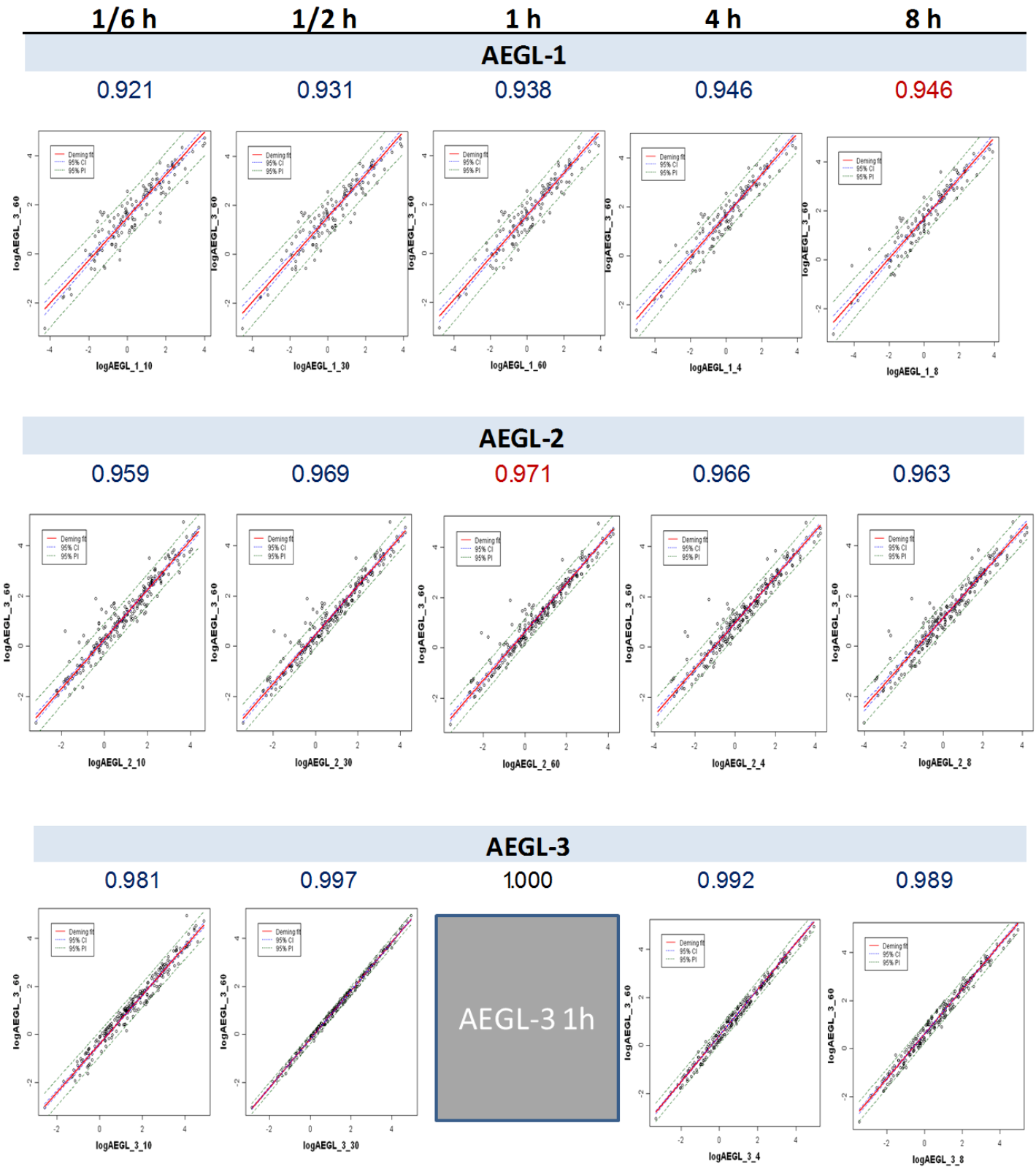


Figure 2 (13 of 15)

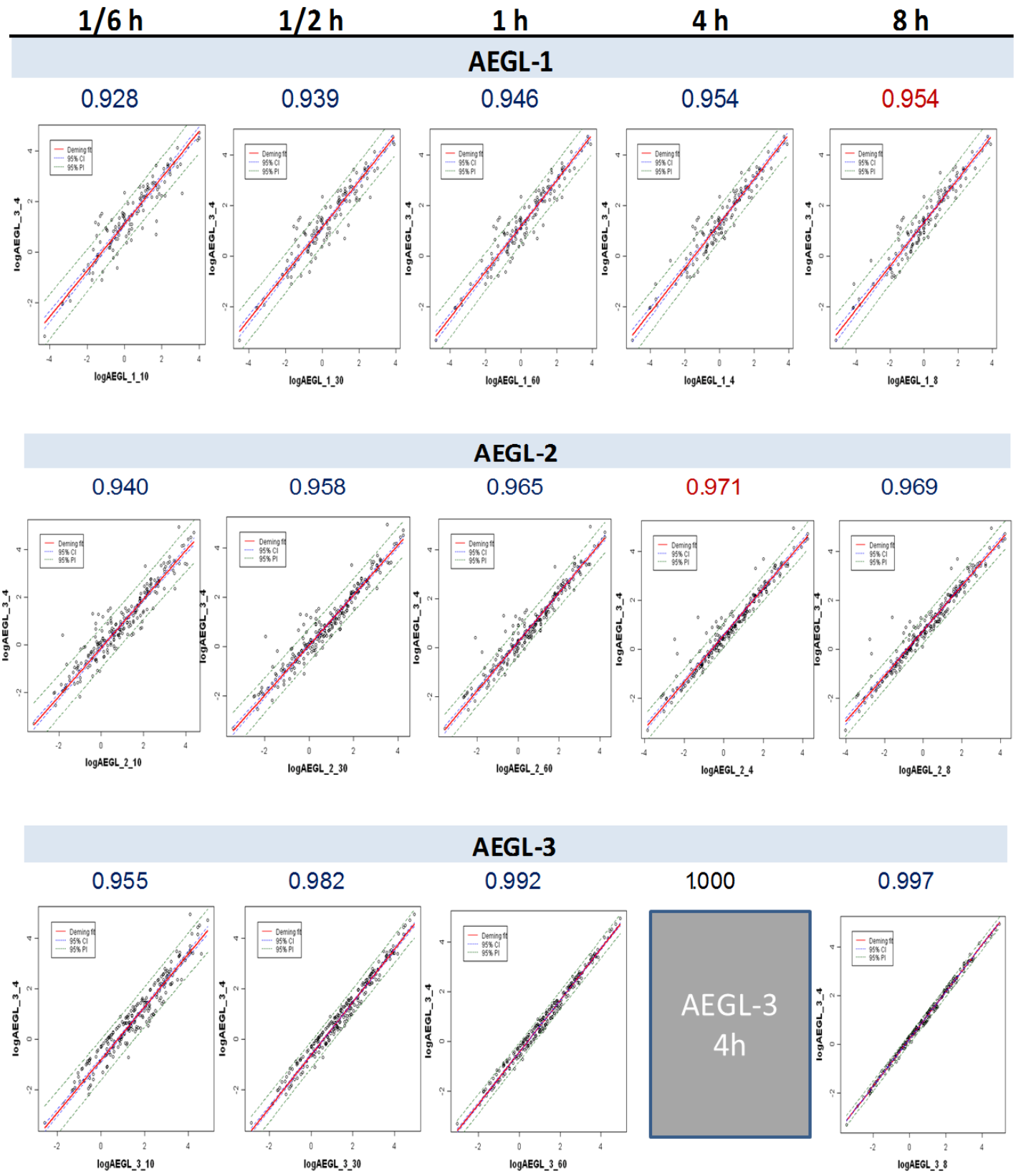


Figure 2 (14 of 15)

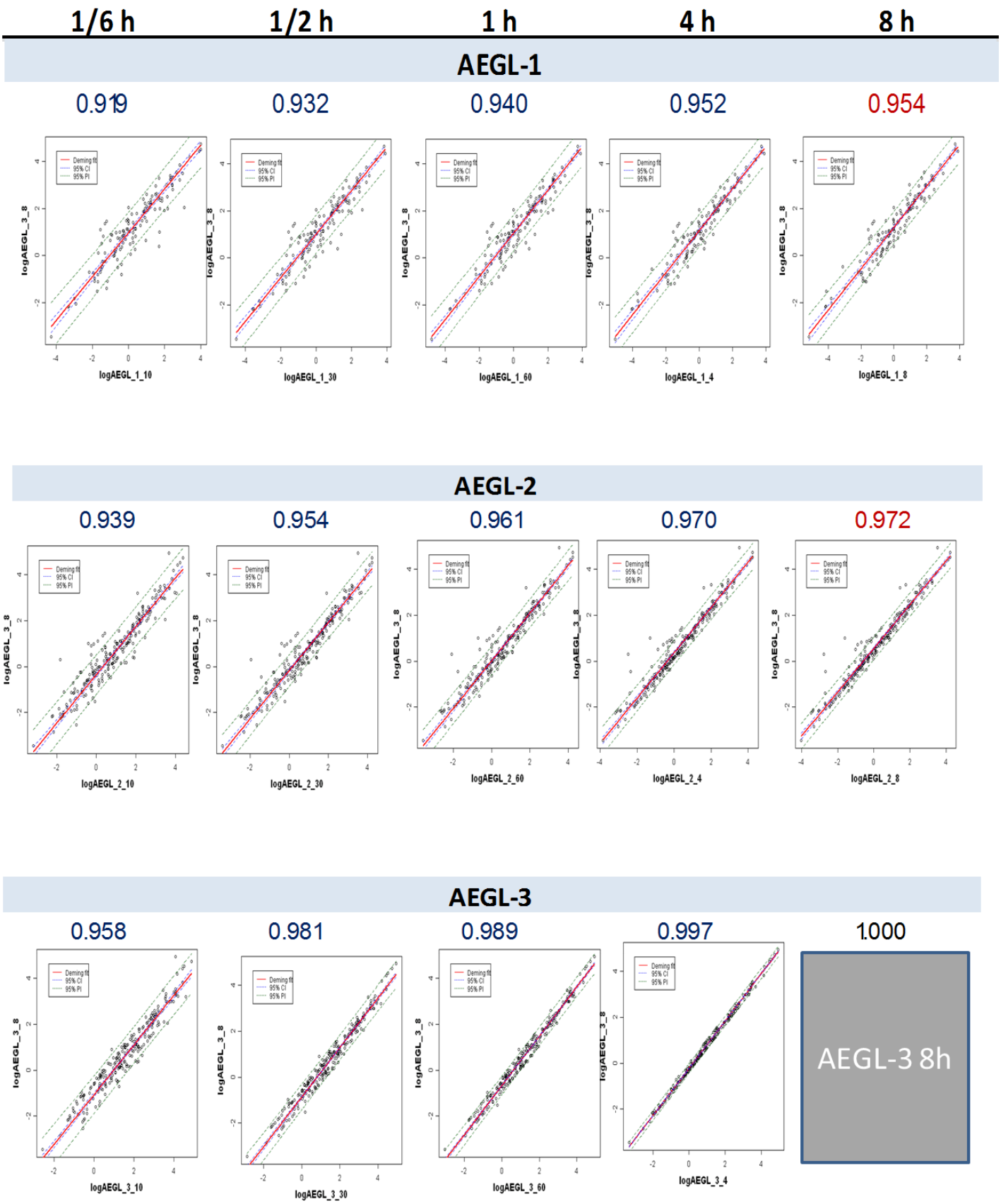


Figure 2 (15 of 15)

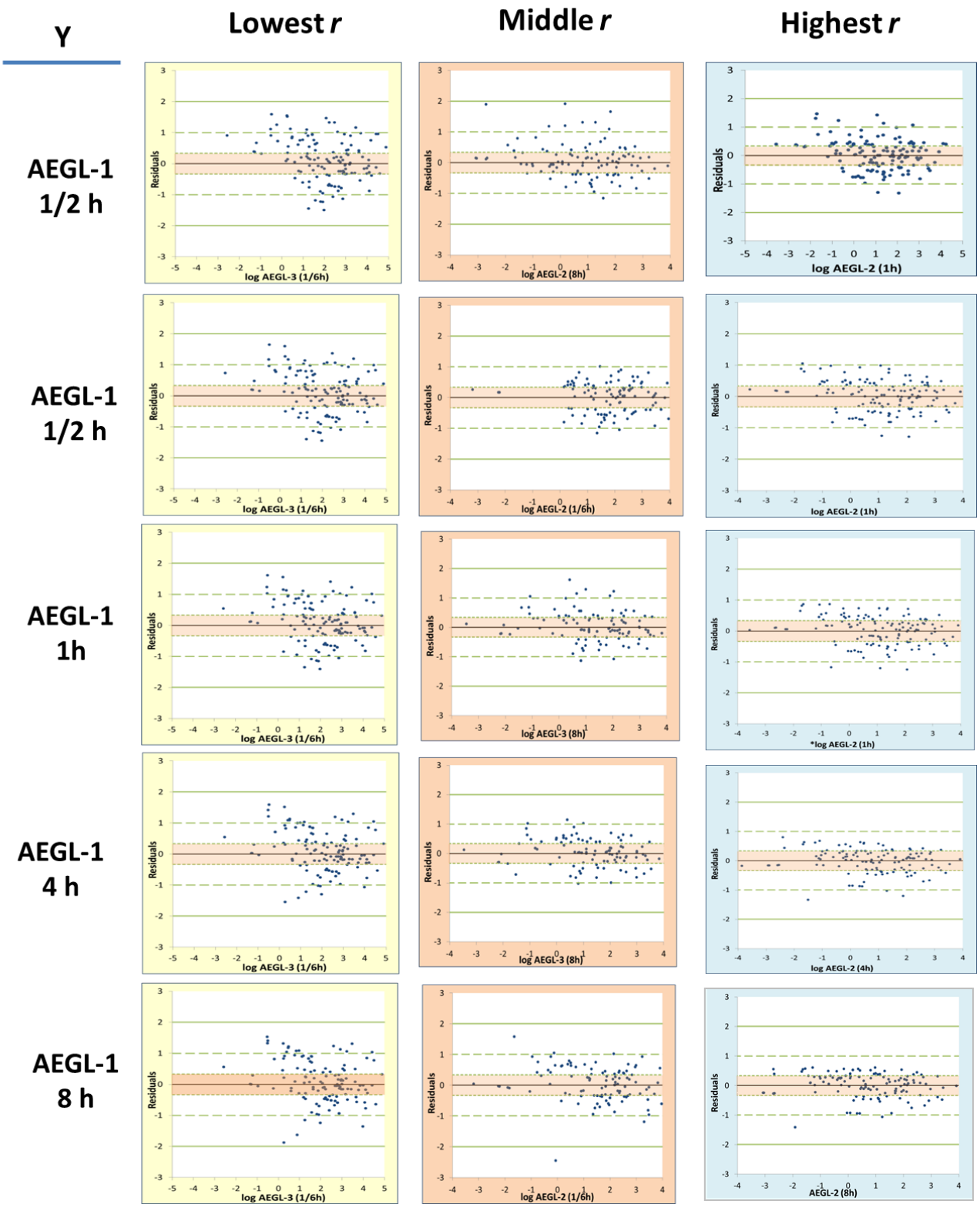


Figure 3. Residual plots of AEGL estimates for the 15 duration-and-threshold-specific AEGL levels. Three AEGL pair models were selected for each, ranked by the magnitude of their correlation coefficients: highest (blue), middle (orange), and lowest (yellow). Normality and proximity of predictions to actual values were assessed by the scatter and distance of the AEGL estimates about the horizontal axis. Horizontal green lines indicate the cut-off levels for the magnitude difference between predicted and actual values: 3, 10, and 100-fold difference.

Figure 3 (1 of 3)

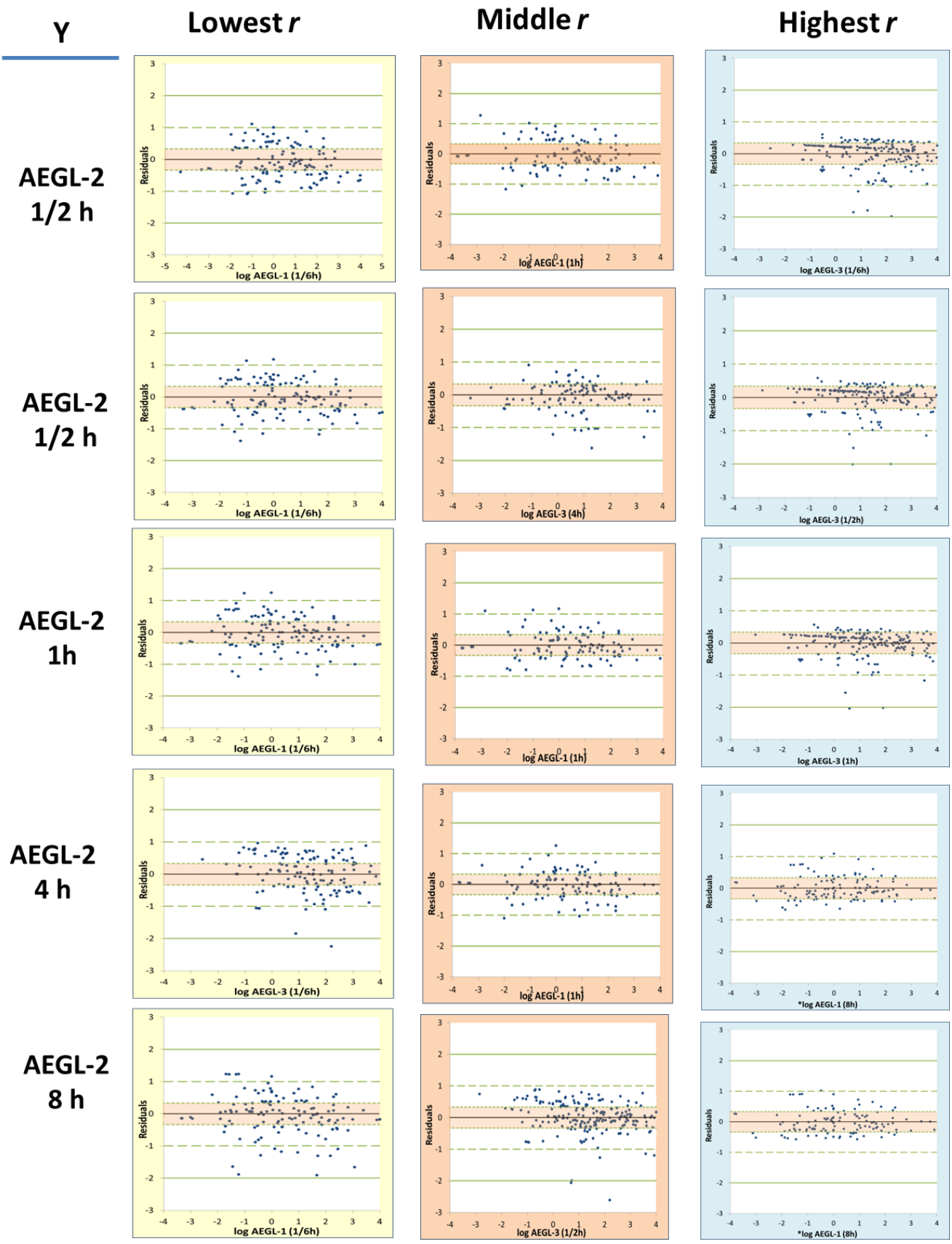


Figure 3 (2 of 3)

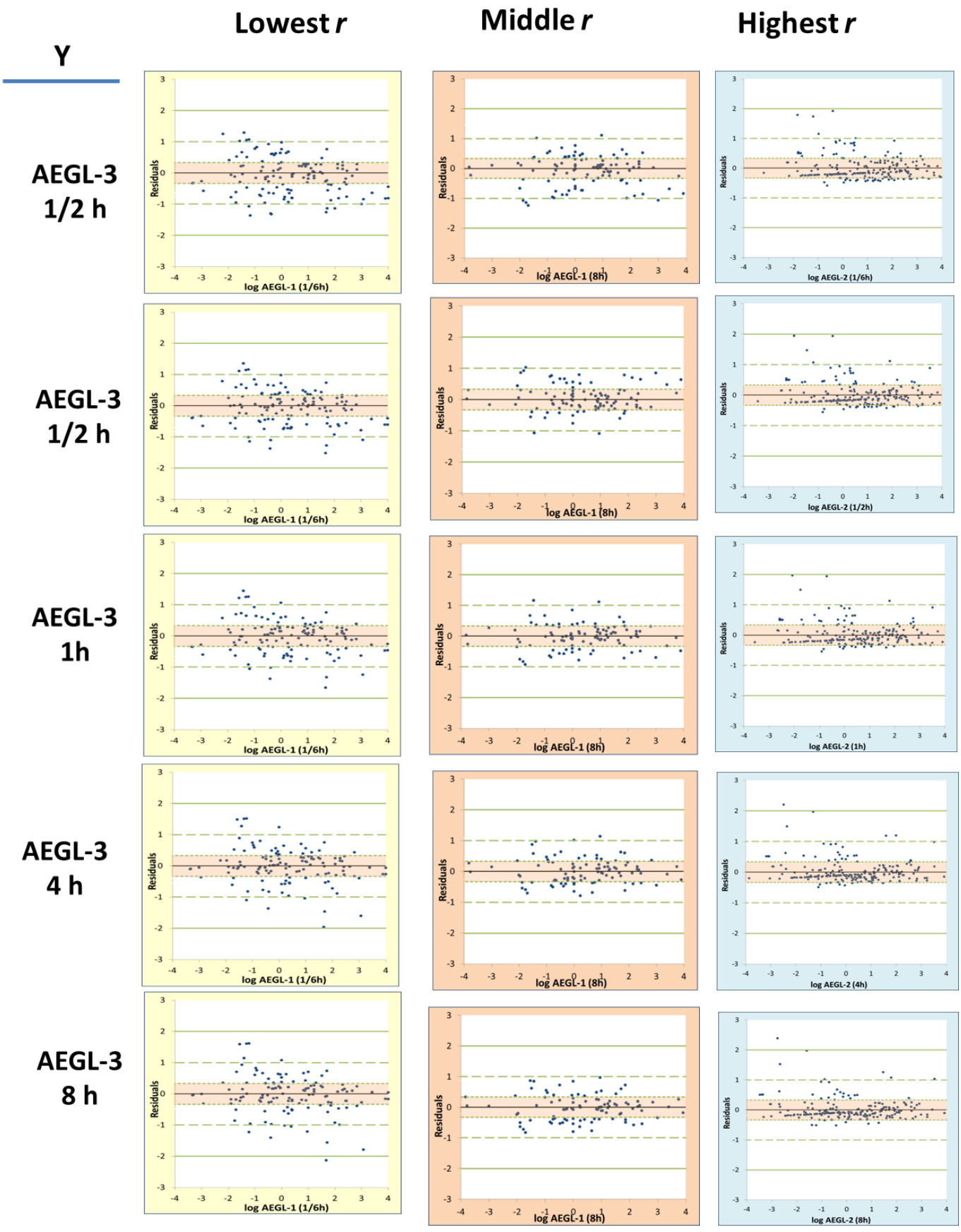


Figure 3 (3 of 3)

	Lowest r					Middle r					Highest r					Narrowest 95% PIs				
Response	Predictor-Lowest	3	10	100	> 100	Predictor-Middle	3	10	100	>100	Predictor-Highest	3	10	100	>100	Predictor-Highest	3	10	100	>100
AEGL-1 1/6h	AEGL-3 1/6h	31.5	52.4	12.5	0.0	AEGL-2 8h	42.3	48.2	9.5	0.0	AEGL-2 1h	48.2	47.0	4.8	0.0	AEGL-2 1h	(same as highest r models)			
AEGL-1 1/2h	AEGL-3 1/6h	32.7	54.3	13.0	0.0	AEGL-2 1/6h	31.5	63.1	5.4	0.0	AEGL-2 1h	52.4	45.8	1.8	0.0	AEGL-2 4h	82.7	17.3	0.0	0.0
AEGL-1 1h	AEGL-3 1/6h	35.2	52.5	12.3	0.0	AEGL-3 8h	60.5	30.2	9.3	0.0	AEGL-2 1h	54.2	44.0	1.8	0.0	AEGL-2 4h	94.8	5.2	0.0	0.0
AEGL-1 4h	AEGL-3 1/6h	37.3	48.7	13.9	0.0	AEGL-3 8h	55.7	38.0	6.3	0.0	AEGL-2 4h	67.9	28.0	1.8	0.0	AEGL-2 4h	*(same as highest r models)*			
AEGL-1 8h	AEGL-3 1/6h	34.2	53.2	12.7	0.0	AEGL-2 1/6h	38.4	57.3	3.7	0.6	AEGL-2 4h	67.9	28.0	1.8	0.0	AEGL-2 4h				
AEGL-2 1/6h	AEGL-1 1/6h	33.9	63.1	3.0	0.0	AEGL-1 1h	42.9	54.8	2.4	0.0	AEGL-3 1/6h	70.6	27.5	1.9	0.0	AEGL-3 1/2h	75.2	22.5	1.5	0.8
AEGL-2 1/2h	AEGL-1 1/6h	36.3	59.5	4.2	0.0	AEGL-3 4h	74.4	21.3	3.9	0.4	AEGL-3 1/2h	76.3	21.4	1.1	0.8	AEGL-3 1h	76.6	21.1	1.9	0.4
AEGL-2 1h	AEGL-1 1/6h	50.6	44.6	4.8	0.0	AEGL-1 1h	57.1	41.1	1.8	0.0	AEGL-3 1h	78.2	20.2	0.8	0.8	AEGL-3 1h	(same as highest r models)			
AEGL-2 4h	AEGL-3 1/6h	39.4	56.4	3.9	0.4	AEGL-1 1h	61.3	36.9	1.8	0.0	AEGL-1 8h	73.2	25.6	1.2	0.0	AEGL-3 4h	80.7	17.0	1.5	0.8
AEGL-2 8h	AEGL-1 1/6h	42.3	48.2	9.5	0.0	AEGL-3 1/2h	58.7	38.2	1.9	0.8	AEGL-1 8h	69.5	29.3	1.2	0.0	AEGL-3 8h	81.5	15.4	2.3	0.8
AEGL-3 1/6h	AEGL-1 1/6h	38.3	53.7	8.0	0.0	AEGL-1 8h	38.0	55.7	6.3	0.0	AEGL-2 1/6h	72.1	26.0	1.9	0.0	AEGL-2 1/6h	(same as highest r models)			
AEGL-3 1/2h	AEGL-1 1/6h	36.4	56.2	7.4	0.0	AEGL-1 8h	62.0	34.2	3.8	0.0	AEGL-2 1/2h	78.2	19.5	1.9	0.0	AEGL-2 1/2h				
AEGL-3 1h	AEGL-1 1/6h	58.6	34.0	7.4	0.0	AEGL-1 8h	62.7	34.2	3.2	0.0	AEGL-2 1h	80.2	18.3	1.5	0.0	AEGL-2 1h				
AEGL-3 4h	AEGL-1 1/6h	63.6	29.0	7.4	0.0	AEGL-1 8h	64.6	31.0	4.4	0.0	AEGL-2 4h	83.2	12.6	2.7	0.4	AEGL-2 4h				
AEGL-3 8h	AEGL-1 1/6h	61.7	29.6	8.0	0.6	AEGL-1 8h	58.9	38.6	2.5	0.0	AEGL-2 8h	84.2	12.7	2.7	0.4	AEGL-2 8h				

Table 7. Test of DLR model performance. AEGL pair models ranked by their Pearson correlations (high, middle, and low) were assessed for the percentage of compounds with AEGLs estimates falling within a magnitude of 3, 10, 100, and >100-folds difference from actual AEGL values. Models with high Pearson correlation coefficients had more compounds with AEGL estimates within a 3-fold difference than for models with the middle and lowest Pearson correlations. Yet, AEGL models with the narrowest 95% PIs, regardless of correlation magnitude, had highest percentage of compounds with estimates within a 3-fold difference.

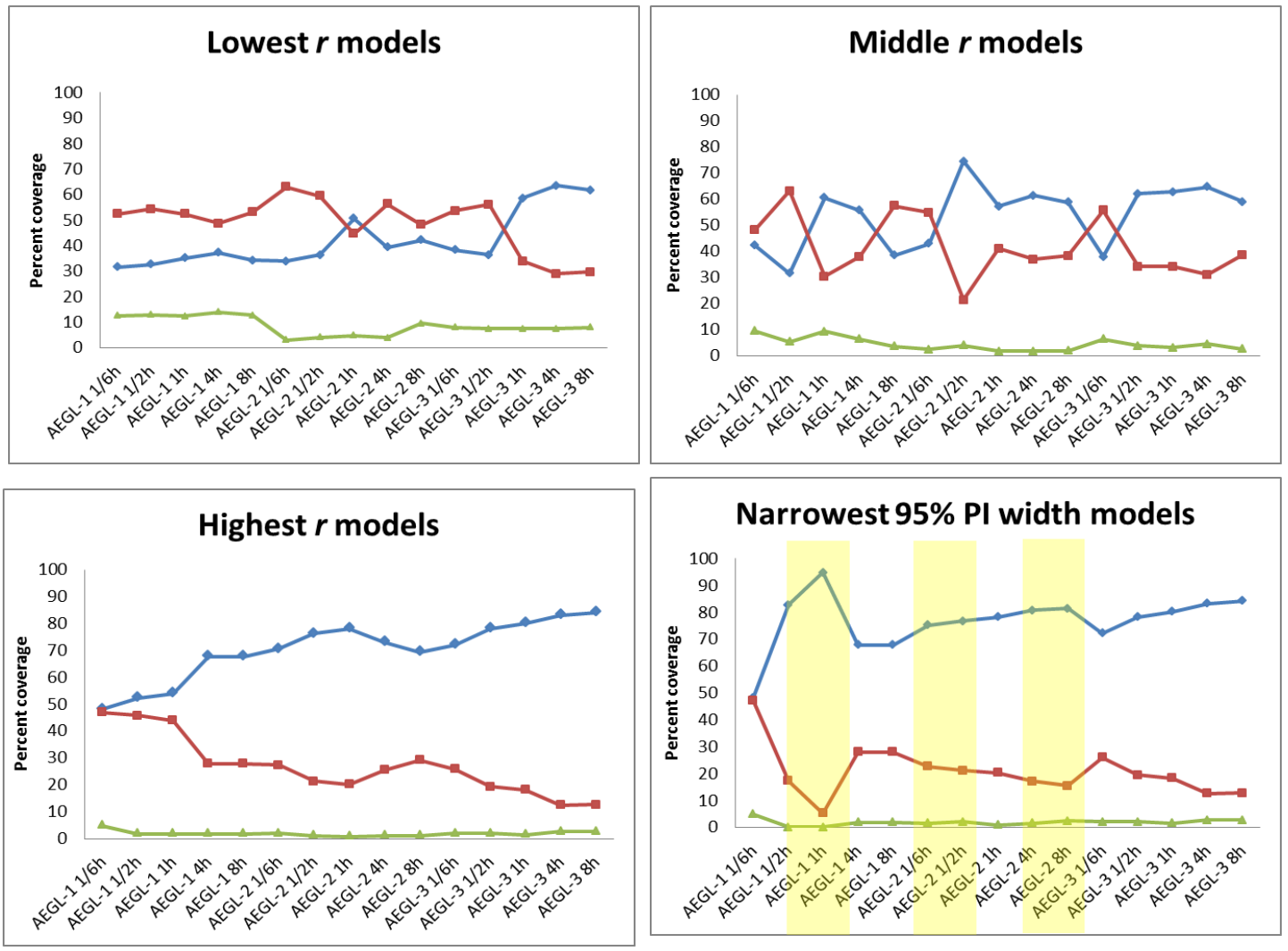


Figure 4. Line graphs of DLR model performance for each AEGL pair models ranked by their Pearson correlations (highest, middle, and lowest). The percentage of compounds with AEGLs estimates falling within a magnitude of 3 (blue), 10 (red), and 100-folds (green) difference from actual AEGLs were assessed. Models with higher Pearson correlation coefficients mostly had more compounds with AEGL estimates within a 3-fold difference. Yet, for 6 models with lower correlations but narrower 95% PI widths (highlighted yellow), the percentage of compounds with AEGL estimates within a 3-fold difference was the highest out of all model types. Although a relationship between Pearson correlations and 95% PI width seems to exist, model performance was observed to be more dependent on 95% PI width.

Best model selection			
Response	#1 Predictor (all)	#2 Predictor (within threshold)	#3 Predictor (cross-threshold)
AEGL-1 1/6h	AEGL-2 1h	NA	AEGL-3 4h
AEGL-1 1/2h	AEGL-2 4h	NA	AEGL-2 1h
AEGL-1 1h	AEGL-2 4h	NA	AEGL-2 1h
AEGL-1 4h	AEGL-2 4h	NA	AEGL-2 1h
AEGL-1 8h	AEGL-2 8h	NA	AEGL-2 1h
AEGL-2 1/6h	AEGL-3 1/2h	AEGL-2 1/2h	AEGL-3 1/6h
AEGL-2 1/2h	AEGL-3 1h	AEGL-2 1h	AEGL-3 1/2h
AEGL-2 1h	AEGL-3 1h	AEGL-2 1/2h	AEGL-3 4h
AEGL-2 4h	AEGL-3 4h	AEGL-2 1h	AEGL-1 8h
AEGL-2 8h	AEGL-3 8h	AEGL-2 1h	AEGL-1 8h
AEGL-3 1/6h	AEGL-2 1/6h	AEGL-3 1/2h	AEGL-2 1/2h
AEGL-3 1/2h	AEGL-2 1/2h	AEGL-3 1h	AEGL-2 1/2h
AEGL-3 1h	AEGL-2 1h	AEGL-3 1/2h	AEGL-2 1/2h
AEGL-3 4h	AEGL-2 4h	AEGL-3 1h	AEGL-3 1h
AEGL-3 8h	AEGL-2 8h	AEGL-3 1h	AEGL-3 1h

Table 8. Selection criteria for the "best" predictive models. AEGL model pairs with the best model performance for each duration-and-threshold-specific AEGL level were ranked by (1) the magnitude difference of their AEGL estimates to actual values, (2) width of their 95% PIs, (3) residual plots, and (4) their Pearson correlation coefficient magnitude. Alternative model pairs, within and cross-threshold, were presented in cases where an AEGL predictive value for the best model is unassigned for a compound.

Overlapping AEGL compounds	NIOSH REL-STEL (1/4h)	NIOSH REL-TWA (10h)	ACGIH TLV-STEL (1/4h)	ACGIH TLV-TWA (8h)
Sulfuryl fluoride	1.00	0.70	1.00	0.70
Carbonyl fluoride	0.70	0.30	0.70	0.30
Iron pentacarbonyl	-0.70	-1.00	-0.70	-1.00
Pentaborane	-1.82	-2.30	-1.82	-2.30
Osmium tetroxide	-3.22	-3.70	-3.22	-3.70
n-Hexane	NA	1.70	NA	1.70
Carbon monoxide	NA	1.54	NA	1.40
Propyleneimine	NA	0.30	NA	0.30
Phosphine	0.00	-0.52	NA	-0.52
Diborane	NA	-1.00	NA	-1.00
Hexafluoroacetone	NA	-1.00	NA	-1.00
Phosgene	NA	-1.00	NA	-1.00
Nickel carbonyl	NA	-3.00	NA	-1.30
Phosphorus oxychloride	-0.30	-1.00	NA	-1.00
Phenol	NA	0.70	NA	0.70
Ethylbenzene	2.10	2.00	2.10	2.00
Ammonia	1.54	1.40	1.54	1.40
Styrene	2.00	1.70	1.60	1.30
Toluene	2.18	2.00	NA	1.30
Perchloryl fluoride	0.78	0.48	0.78	0.48
Nitric Acid	0.60	0.30	0.60	0.30
Benzene	0.00	-1.00	0.40	-0.30
Ketene	0.18	-0.30	0.18	-0.30
Phosphorus Trichloride	-0.30	-0.70	-0.30	-0.70
Bromine	-0.52	-1.00	-0.70	-1.00
Carbon tetrachloride	0.30	NA	1.00	0.70
Nitrogen dioxide	0.00	NA	0.70	0.48
Acetone	NA	2.40	2.88	2.70
Cumene	NA	1.70	NA	1.70
Cyanogen	NA	1.00	NA	1.00
Cyclohexylamine	NA	1.00	NA	1.00
Nitrogen trifluoride	NA	1.00	NA	1.00
Dimethylamine	NA	1.00	1.18	0.70
Methylamine	NA	1.00	1.18	0.70
Acrylicacid	NA	0.30	NA	0.30
Acrylonitrile	NA	0.00	NA	0.30
Allyl chloride	0.30	0.00	NA	0.00
Carbon disulfide	1.00	0.00	NA	0.00
Fluorine	NA	-1.00	0.30	0.00
Propargyl alcohol	NA	0.00	NA	0.00
Allyl alcohol	0.60	0.30	NA	-0.30
Hydrogen fluoride	NA	0.48	NA	-0.30
Chloroacetylchloride	NA	-1.30	-0.82	-1.30
Propylene glycol dinitrate	NA	-1.30	NA	-1.30

Table 9. Compounds in the AEGL database with NIOSH and ACGIH's occupational exposure limits (OEL) assigned. Compounds highlighted in red have unassigned AEGL-1 values (NA = not available).

Deming comparisons	X	Y	Intercept	Slope	95% CI LL	95% CI UL	Correlation
OELs vs OELs	NIOSH REL-STEL (1/4 h)	ACGIH TLV-STEL (1/4 h)	-0.01	0.98	0.91	1.05	0.99
	NIOSH REL-TWA (10h)	NIOSH REL-STEL (1/4 h)	0.37	0.93	0.86	1.00	0.99
	NIOSH REL-TWA (10h)	ACGIH TLV-STEL (1/4 h)	0.36	0.91	0.80	1.04	0.98
	ACGIH TLV-TWA (8 h)	NIOSH REL-STEL (1/4 h)	0.40	0.97	0.89	1.05	0.99
	ACGIH TLV-TWA (8 h)	NIOSH REL-TWA (10h)	0.03	1.04	0.93	1.16	0.98
	ACGIH TLV-TWA (8 h)	ACGIH TLV-STEL (1/4 h)	0.34	0.94	0.89	1.00	1.00
STELs vs AEGLs	AEGL-2 8h	ACGIH TLV-STEL	0.01	0.79	0.54	1.12	0.86
	AEGL-2 4h	ACGIH TLV-STEL	-0.15	0.82	0.57	1.17	0.85
	AEGL-1 8h	ACGIH TLV-STEL	0.54	0.73	0.43	1.16	0.85
	AEGL-2 1h	ACGIH TLV-STEL	-0.38	0.85	0.56	1.25	0.83
	AEGL-1 4h	ACGIH TLV-STEL	0.49	0.72	0.39	1.19	0.83
TWAs vs AEGLs	*AEGL-2 8h	ACGIH TLV-TWA	-0.30	0.77	0.63	0.92	0.86
	AEGL-2 8h	NIOSH REL-TWA	-0.36	0.87	0.71	1.06	0.86
	*AEGL-2 4h	ACGIH TLV-TWA	-0.47	0.80	0.66	0.97	0.85
	AEGL-2 4h	NIOSH REL-TWA	-0.56	0.91	0.74	1.11	0.85
	AEGL-1 8h	ACGIH TLV-TWA	0.02	0.89	0.69	1.14	0.84
	AEGL-1 4h	ACGIH TLV-TWA	-0.04	0.89	0.67	1.17	0.82
	** statistical significance of the slope*						

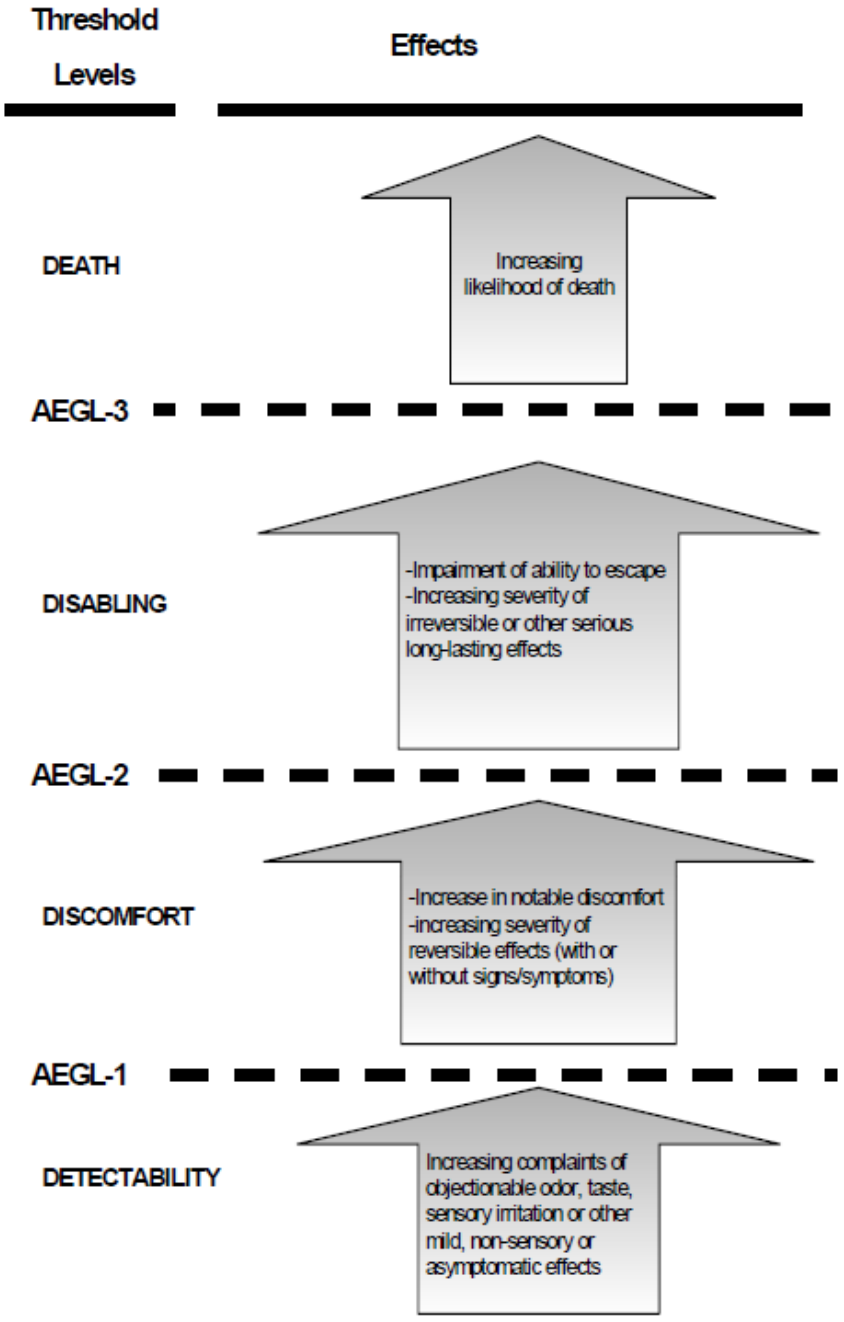
Table 10. Deming linear regression assessment of data comparability within OELs, and between OELs and assigned AEGL values. Comparisons of OELs with each other showed statistical identity of slopes (95% CI contain 1) for all OEL pairs. Comparisons of OEL-STELs with AEGLs showed all pairs had statistically identical slopes, and that the highest correlated pairs were between OEL-STELs and AEGL-1s and -2s at the 4 h and 8 h, and AEGL-2 at 1 h. Comparisons between OEL-TWAs and AEGLs showed statistical identity for all pairs except for ACGIH TLV-TWAs and AEGL-2s at the 4 and 8h. The highest correlation also existed between OEL-TWA pairs with AEGL-1s and -2s at the 4 h and 8 h. The statistical identity in slopes of OELs especially with AEGL-1s at the 4 h and 8 h exposure durations (highlighted in red) indicate that their data are comparable. Hence, OEL values can then be used as a crude external validation for DLR derived AEGL-1 estimates at 4h and 8h for compounds with unassigned values.

AEGL Deming regression model	X: AEGL-1 4h, Y=AEGL-2 4h			X: AEGL-1 8h, Y=AEGL-2 8h			X: AEGL-2 4h, Y=AEGL-3 4h			X: AEGL-2 8h, Y=AEGL-3 8h			*Extermal cross-reference*			*Internal cross-reference*	
	Est	2.5% PI LL	97.5% PI UL	Est	2.5% PI LL	97.5% PI UL	Est	2.5% PI LL	97.5% PI UL	Est	2.5% PI LL	97.5% PI UL	ACGIH TLV-STEL (1/4h)	NIOSH REL-TWA (10h)	ACGIH TLV-TWA (8h)	Actual AEGL-2 4h	Actual AEGL-2 8h
Sulfuryl fluoride	0.39	-0.20	0.98	0.16	-0.45	0.78	1.07	0.55	1.59	0.78	0.27	1.30	1.00	0.70	0.70	1.11	0.83
Carbonyl flouride	-1.60	-2.22	-0.98	-1.82	-2.47	-1.18	-0.90	-1.43	-0.36	-1.20	-1.72	-0.67	0.70	0.30	0.30	-0.77	-1.06
Iron pentacarbonyl	-2.30	-2.94	-1.65	-2.39	-3.06	-1.74	-1.60	-2.15	-1.04	-1.76	-2.30	-1.22	-0.70	-1.00	-1.00	-1.43	-1.60
Pentaborane	-2.18	-2.81	-1.54	-2.34	-3.01	-1.68	-1.25	-1.79	-0.70	-1.48	-2.01	-0.94	-1.82	-2.30	-2.30	-1.32	-1.55
Osmium Tetroxide	-3.41	-4.09	-2.72	-3.62	-4.34	-2.92	-0.19	-0.71	0.34	-0.27	-0.78	0.25	-3.22	-3.70	-3.70	-2.48	-2.77
n-Hexane	2.93	2.31	3.56	3.00	2.34	3.66	4.55	3.95	5.14	4.60	3.99	5.20	NA	2.00	1.70	3.52	3.52
Carbon monoxide	0.82	0.23	1.41	0.89	0.27	1.51	1.67	1.15	2.19	1.64	1.12	2.15	NA	1.54	1.40	1.52	1.43
Propyleneimine	-0.37	-0.96	0.23	-0.62	-1.25	0.00	0.14	-0.38	0.66	-0.18	-0.69	0.33	NA	0.30	0.30	0.40	0.08
Phosphine	-0.47	-1.06	0.13	-1.34	-1.98	-0.71	-0.65	-1.18	-0.11	-0.73	-1.26	-0.20	NA	-0.52	-0.52	-0.30	-0.60
Diborane	-1.42	-2.04	-0.80	-1.64	-2.28	-1.00	-0.64	-1.17	-0.10	-0.94	-1.46	-0.41	NA	-1.00	-1.00	-0.60	-0.89
Hexafluoroacetone	-2.16	-2.80	-1.52	-2.39	-3.06	-1.74	0.76	0.24	1.28	0.47	-0.04	0.98	NA	-1.00	-1.00	-1.30	-1.60
Phosgene	-1.95	-2.57	-1.31	-2.18	-2.84	-1.53	-1.33	-1.87	-0.78	-1.68	-2.22	-1.14	NA	-1.00	-1.00	-1.10	-1.40
Nickel carbonyl	-2.95	-3.61	-2.28	-3.18	-3.87	-2.49	-2.06	-2.62	-1.49	-2.37	-2.92	-1.81	NA	-3.00	-1.30	-2.05	-2.35
Phosphorous oxychloride	-1.78	-2.59	-0.98	-1.87	-2.71	-1.03	-0.88	-1.41	-0.34	-1.10	-1.68	-0.53	NA	-1.00	-1.00	NA	NA

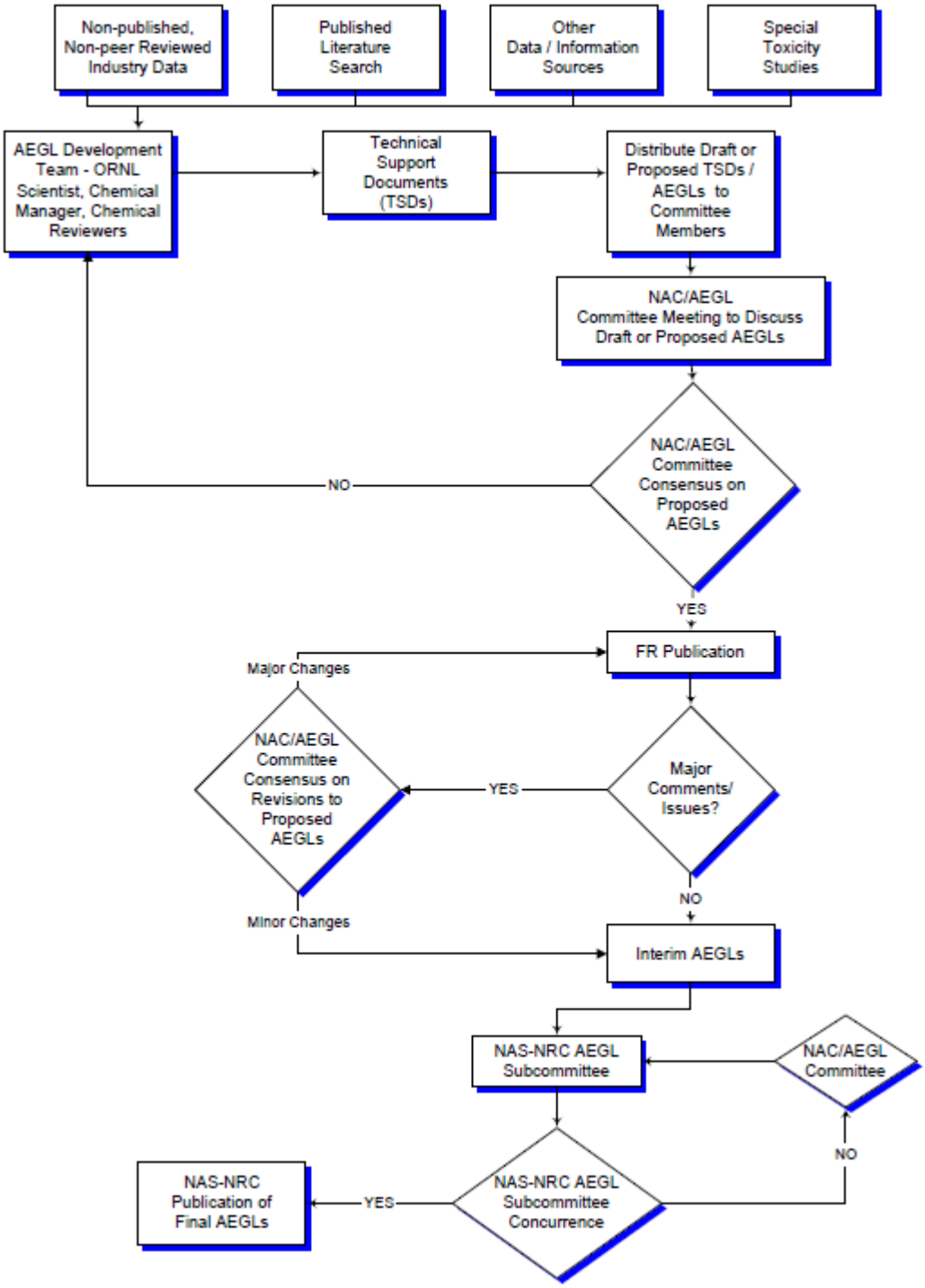
Table 11. Internal and external cross-validation of AEGL estimates from the proposed "best" DLR models. For the 14 compounds with unassigned AEGL-1 values, AEGL-1 and -2 estimates at the 4 h and 8 h exposure duration were derived from the best DLR model pairs. These estimates were compared to OEL and known AEGL-2 values to assess validity of model estimates for the respective compounds. For each of the 4 DLR models employed, X = AEGL predictor value for DLR model and Y = AEGL-1s or -2s at the 4 h or 8 h durations. AEGL-1 estimates were assumed to be statistically valid if their 95% PIs included the OEL value for each compound (highlighted blue or green cells). At the 95% prediction level, 8/14 compounds had statistically similar estimates between AEGL-1 and OEL-TWA values and 3/14 compounds had statistically similar estimates between AEGL-1 and OEL-STEL values.

IV. APPENDIX

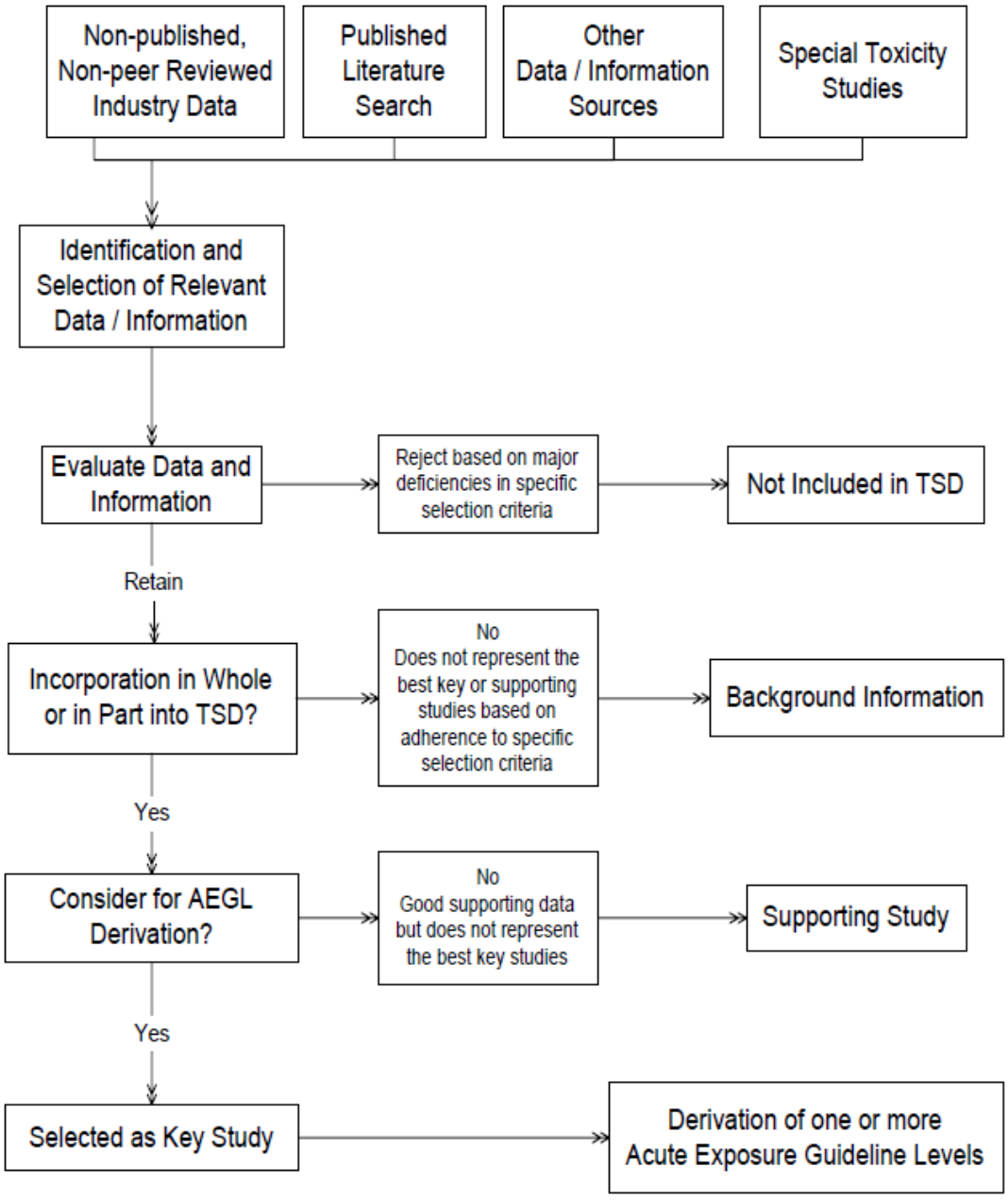
Appendix 1. Hazard assessment (NAS 2001).



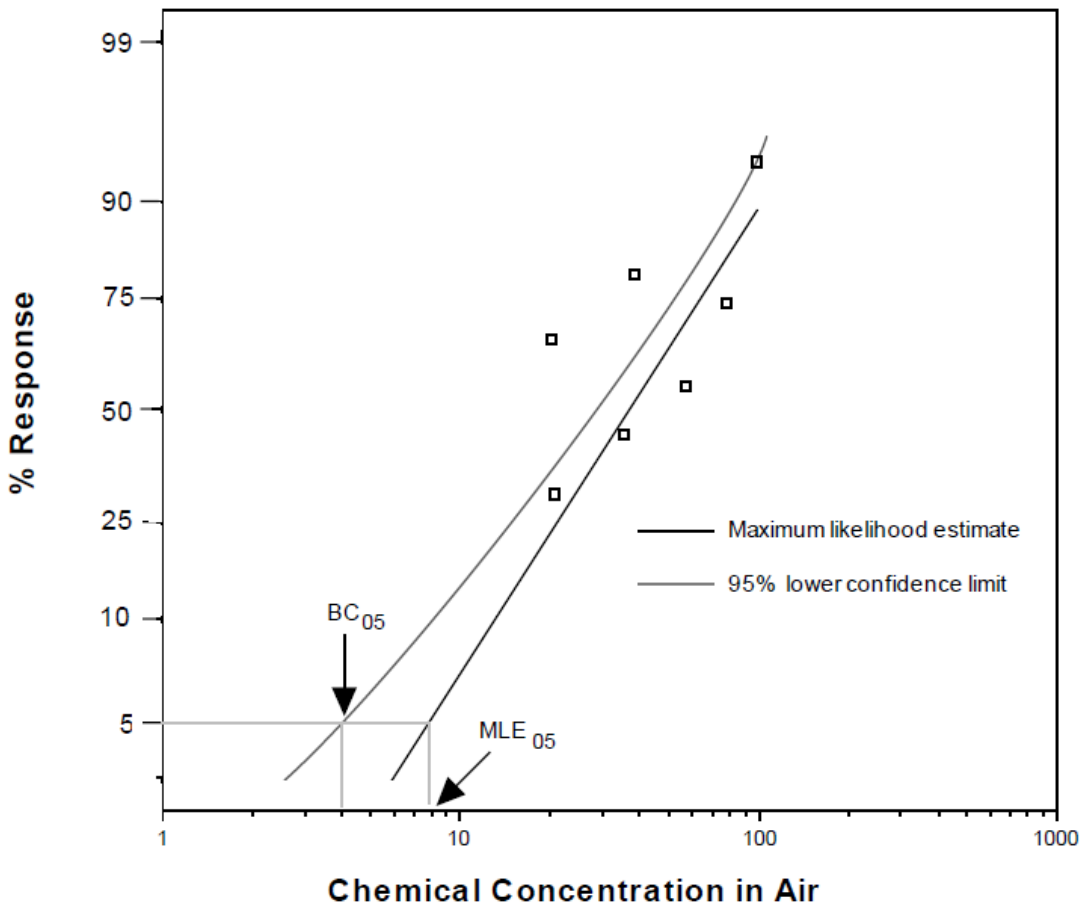
Appendix 2. The AEGL development process (NAS 2001).



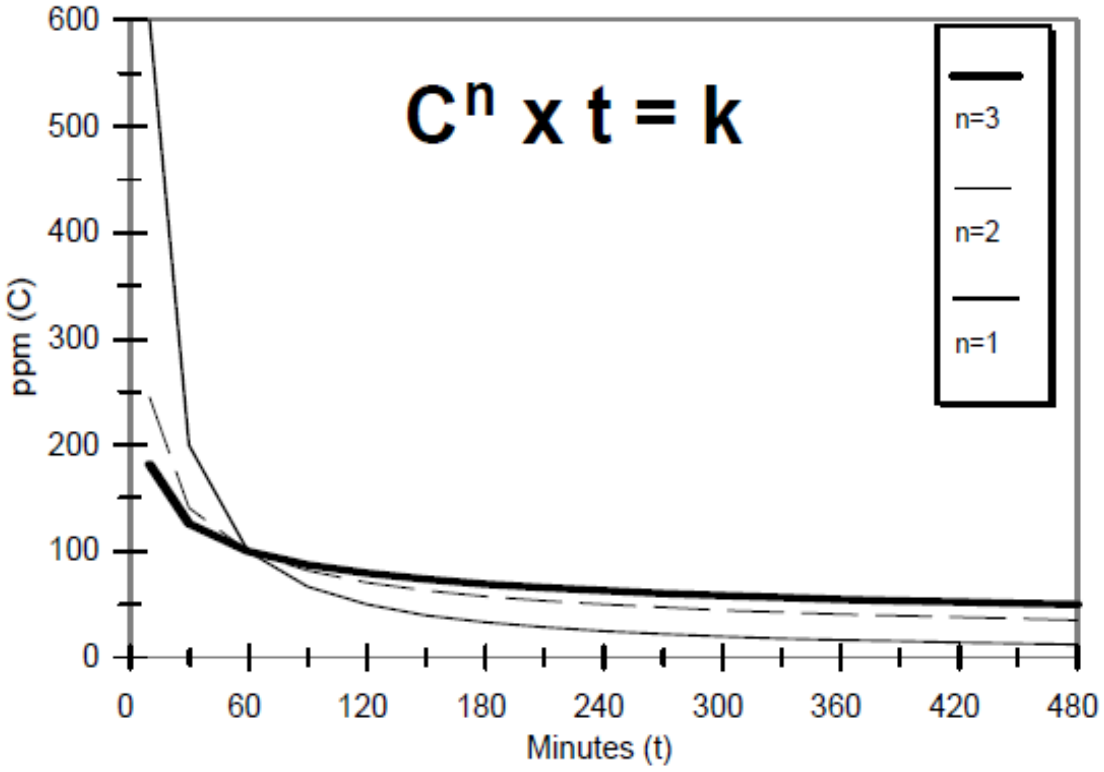
Appendix 3. Decision tree for the selection of key and supporting studies (NAS 2001).



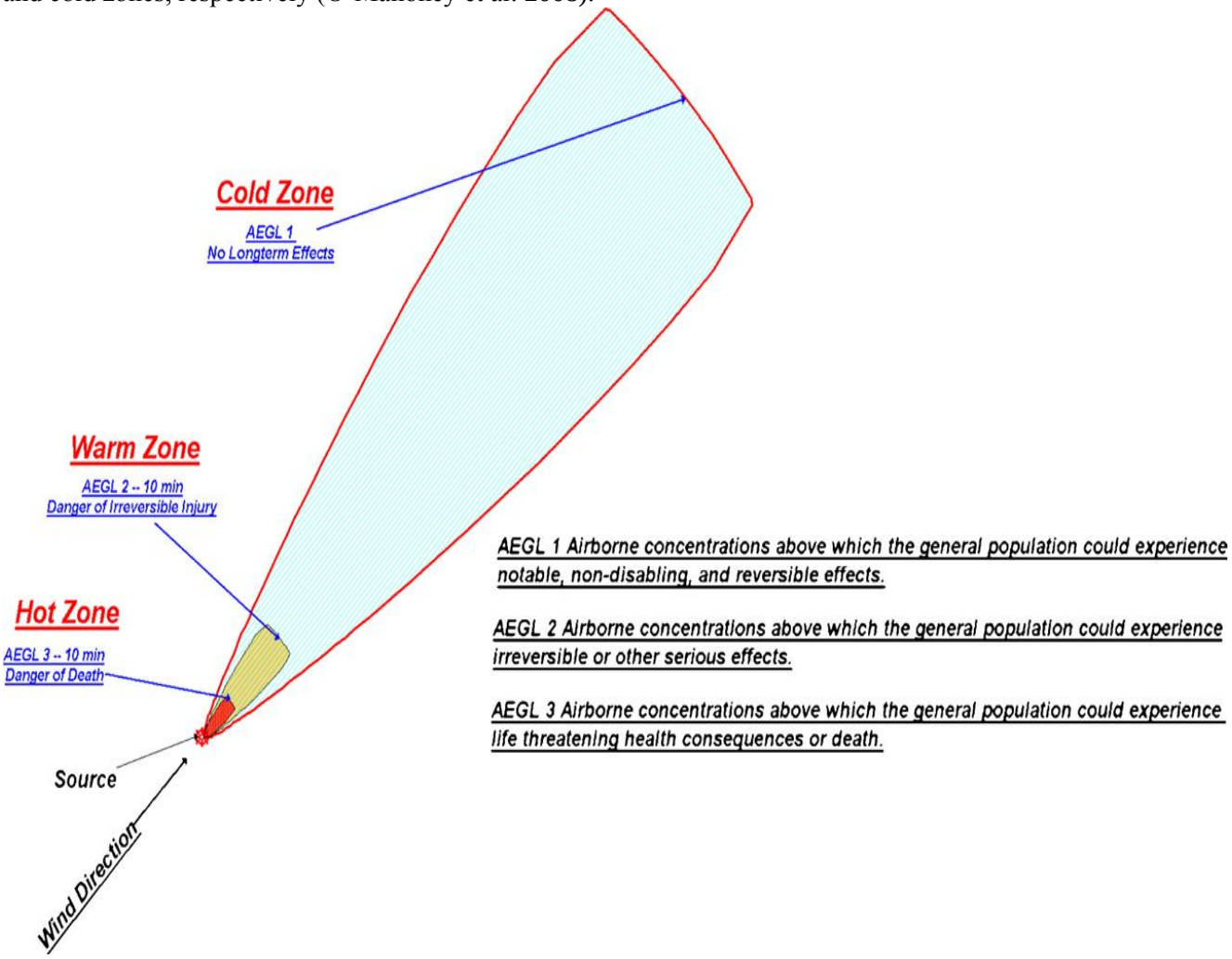
Appendix 4. Log-probit modeling of dose-response data. A benchmark concentration (BMC) estimated for a 5% increase in response (MLE_{05}) (CA EPA, 1999).



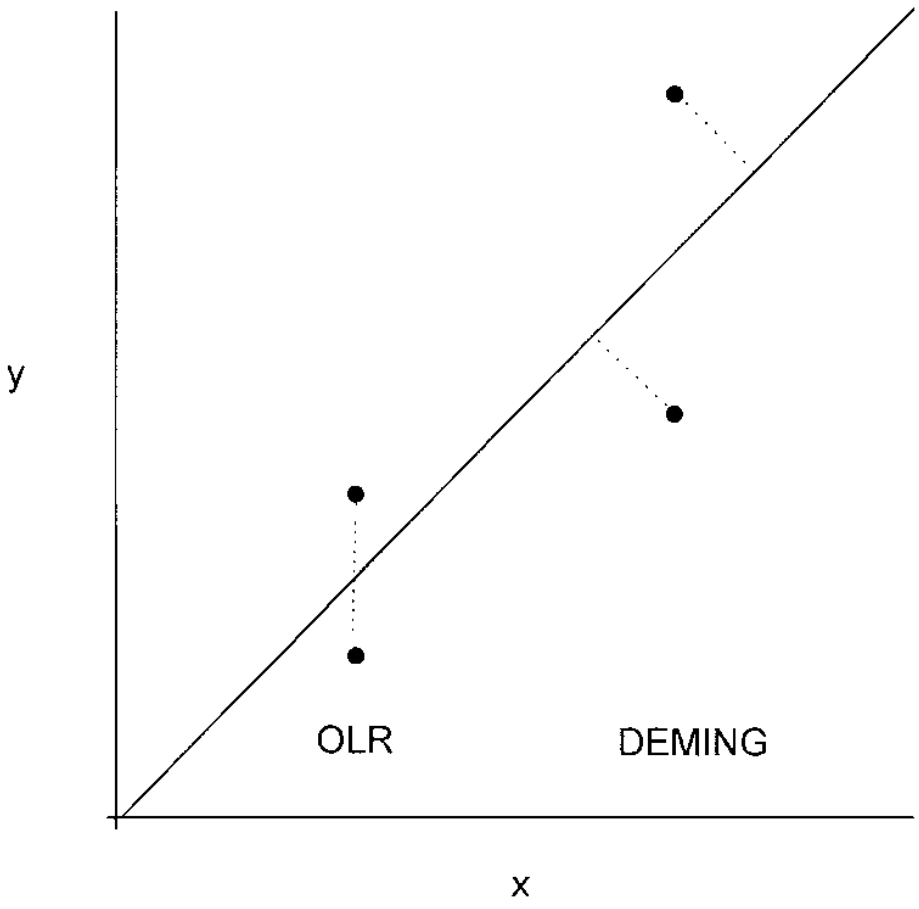
Appendix 5. Influence of n on exposure-duration extrapolations. It is recommended that extropolations from short-to-long exposure durations use an n of 1 and from long-to-short exposure durations use an n of 3 to yield the most conservative concentration estimates (NAS 2001).



Appendix 6. A proposed methodology for applying AEGLs in responding to toxic clouds, based on distance to source: The 10 min AEGL-3, AEGL-2, and AEGL-1 will delimit the hot, warm, and cold zones, respectively (O'Mahoney et al. 2008).



Appendix 7. Difference in errors estimation for OLR and Deming linear regressions (Linnet 1998).



Appendix 8. Deming regression equations used in SAS Macro and R bootstrapping (Linnet 1998).

ESTIMATION OF THE DEMING REGRESSION LINE

In situations with constant analytical errors, i.e., analytical SDs that are independent of the measurement level, the unweighted form of Deming regression analysis is appropriate. The procedure relies on computations of sums of squared deviations and cross-products:

$$x_m = \Sigma x_i/N; y_m = \Sigma y_i/N$$

$$u = \Sigma(x_i - x_m)^2; q = \Sigma(y_i - y_m)^2$$

$$p = \Sigma(x_i - x_m)(y_i - y_m)$$

The subscript m refers to the mean of the variable.

In case of duplicate sets of measurements each x_i and y_i represent the mean of individual measurements ($x_i = (x_{1i}+x_{2i})/2$ and $y_i = (y_{1i}+y_{2i})/2$). Analytical standard deviations for methods x and y are estimated as:

$$SD_{ax}^2 = (1/2N)\Sigma(x_{2i} - x_{1i})^2 \; SD_{ay}^2 = (1/2N)\Sigma(y_{2i} - y_{1i})^2$$

and

$$\lambda = SD_{ax}^2/SD_{ay}^2$$

The Deming regression line is estimated as:

$$b = [(\lambda q - u) + [(u - \lambda q)^2 + 4\lambda p^2]^{0.5}]/2\lambda p$$

$$a = y_m$$

$$Y_{esti} = a + b(x_{esti} - x_m) = a_0 + bX_{esti}; a_0 = a - bx_m$$

X_{esti} and Y_{esti} refer to estimated target values.

Standard errors of a_0 and b are estimated on the basis of a resampling principle, the so-called jackknife procedure *(8)*.

Appendix 9. SAS Macro for Deming Regression (Deal et al. 2011)

dataset = the name of the dataset which contains the paired observations.
id = the name of the variable that contains the subject ids.
method1 = the name of the variable that contains AEGL values from the first duration-and-threshold-specific AEGL level.
Method2 = the name of the variable that contains AEGL values from the first duration-and-threshold-specific AEGL level

%DEMING macro: This macro applies Linnet's Deming equations (Linnet 1998) to the duration-and-threshold-specific AEGL pairs to produce respective slopes and intercepts.

%DOIT macro: This macro calls in the *%DEMING* macro for the entire AEGL database to obtain regression estimates. Jackknife leave-one-out resampling procedure is then applied to generate a new dataset of up to 273 iterations of the slopes and intercepts. This dataset is then used to calculate mean standard errors and subsequently mean 95% confidence intervals for the regression parameters. The significance level was set to 0.05. The *DATA* step and *PROC SQL* procedures then call in the results of the *%DOIT* macro to create a RESULTS dataset containing the slopes, intercepts, their respective standard errors and confidence intervals. Results were also exported to Microsoft Excel [Linnet equations and SAS Macro code in Appendix] (Deal et al. 2011).

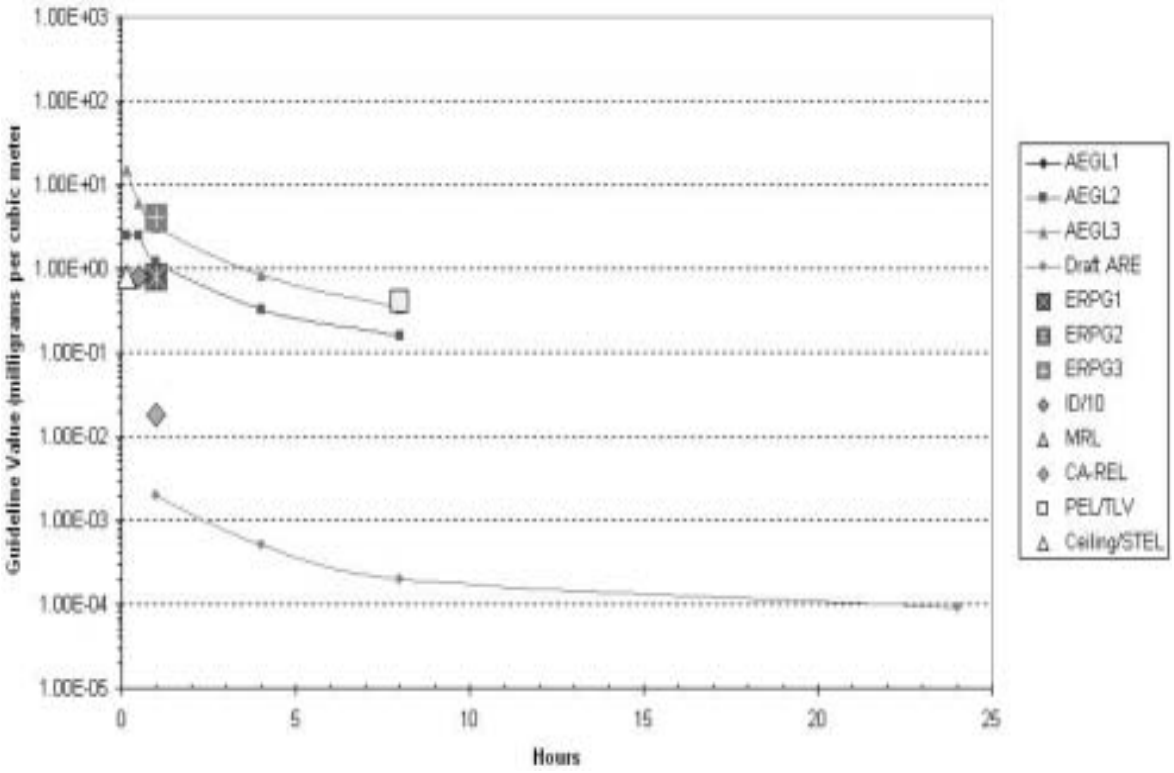
```
/*Create example dataset*/
data example;
      do myid=1 to 200;
            value=UNIFORM(0)*10;
            new=value + NORMAL(0);
            gold=value + NORMAL(1);
            output;
      end;
run;

/*Create %DEMING macro*/
%MACRO DEMING(dataset, id, method1, method2);

      ************************Deming Regression**************************;
      ****************************Linnet 1998*****************************;
      data deming;
            set &dataset;
            keep &id &method1 &method2;
            rename &method2=x &method1=y &id=id;
      run;

      /*Use PROC MEANS to obtain the average measured value for each of the
        two measurement methods across all measured items*/
      proc means data=deming mean NOPRINT;
            var x y;
            output out=means;
      run;
      data _null_;
            set means;
            where  STAT  IN ("MEAN");
            call symputx("x_mean",round(x,0.001));
            call symputx("y_mean",round(y,0.001));
      run;

      /*Calculate sum of squares using a DATA STEP to calculate the squared
        deviations and PROC MEANS to sum those deviations*/
      data deming1;
            set deming;
            u=(x-&x_mean);
            u2=u**2;
            q=(y-&y_mean);
            q2=q**2;
            p=u*q;
      run;
      proc means data=deming1 sum NOPRINT;
            var u2 q2 p;
            output out=means sum=u q p;
      run;
      data _null_;
            set means;
            call symputx("u",round(u,0.001));
            call symputx("q",round(q,0.001));
            call symputx("p",round(p,0.001));
      run;

      /*Use the sum of squares and means obtained above to calculate the
        Deming regression slope and intercept estimates, based on equations
        from Linnet 1998*/
      data deming2;
            b=((&q - &u) + ((&u-&q)**2 + 4*(&p)**2)**0.5)/(2*&p);
```

```
            a0=&y_mean - b*&x_mean;
            dummy=1;
      run;
%MEND DEMING;

/*Create %DOIT macro*/
%MACRO DOIT(dataset, id, method1, method2);

      ********************************************************************************;
      * Step 1: DEMING REGRESSION ESTIMATES
      * Obtain the Deming regression slope and intercept estimates by calling
      * the %DEMING macro on the full dataset
      ********************************************************************************;

      %DEMING(&dataset, &id, &method1, &method2)

      data estimates;
            set deming2;
            rename b = b_est
                   a0 = a0_est;
      run;

      ********************************************************************************;
      * Step 2: JACKKNIFE PROCEDURE
      * Obtain the Deming regression slope and intercept estimates for each of
      * the N datasets created by removing the ith observation from the full
      * dataset and then calling the %DEMING macro on each of those N datasets
      * (based on Linnet 1990)
      ********************************************************************************;

      /*Create a variable containing the number of observations in the full
        dataset*/
      proc means data=&dataset n NOPRINT;
            var &method1;
            output out=n;
      run;
      data  null ;
            set n;
            where _STAT_ IN ("N");
            call symputx("n",round(&method1,0.001));
      run;

      /*Number the N observations in the full dataset 1 thru N*/
      data jackorig;
            set &dataset;
            count+1;
      run;

      /*Create an empty dataset that will hold the results of the jackknife
        procedure*/
      data jack;
            set _null_;
      run;

      /*Call the %DEMING macro N times*/
      %DO i=1 %TO &n;

            /*On the ith iteration, remove the ith observation from the
              original dataset*/
            data jack&i;
                  set jackorig;
```

```
            where count NE &i;
      run;

      /*Call the %DEMING macro on the subsetted dataset*/
      %DEMING(jack&i, &id, &method1, &method2)

      /*Add the Deming regression slope and intercept estimates for the
        ith iteration as the ith observation in the dataset JACK and
        define the variable JACK equal to the value of i*/
      data jack;
            set jack deming2(in=a);
            if a then jack = &i;
            dummy = 1;
      run;

%END;

*************************************************************************;
* Step 3: CONFIDENCE INTERVALS
* Using results from the jackknife procedure and the Deming regression
* slope and intercept estimates, calculate the standard errors of the
* Deming regression slope and intercept estimates and use those to
* produce 95% confidence intervals
*************************************************************************;

/*Calculate the jackknifed estimators of the slope and intercept using a
  a DATA STEP to calculate the estimators for the ith iteration and PROC
  MEANS to obtain the means of those estimators*/
data jackcalc;
      merge jack estimates;
      by dummy;
      jackb=(&n * b_est) - ((&n-1)*b);    /*See Equation 3a*/
      jacka=(&n * a0_est) - ((&n-1)*a0); /*See Equation 3a*/
      call symputx("b_est", b_est);
      call symputx("a0_est", a0_est);
run;
proc means data=jackcalc mean NOPRINT;
      var jackb jacka;
      output out=jackcalc1 mean=jackbmean jackamean;
run;

data jackcalc1;
      set jackcalc1 (drop= _type_ _freq_);
      dummy=1;
run;

/*Calculate the variances of the Deming regression slope and intercept
  estimates using a DATA STEP to calculate the variances for the ith
  ith iteration and PROC MEANS to obtain the sum of those variances*/
data jackcalc2;
      merge jackcalc jackcalc1;
      by dummy;
      diff_b2=(jackb- jackbmean)**2/(&n-1);
      diff_a2=(jacka- jackamean)**2/(&n-1);
run;
proc means data=jackcalc2 sum NOPRINT;
      var diff_b2 diff_a2;
      output out=variance sum=sumb suma;
run;

/*Calculate the standard errors and 95% confidence intervals for the
```

```
        Deming regression slope and intercept estimates*/
      data variance2;
            set variance;
            se_b=SQRT(sumb/&n);
            se_a=SQRT(suma/&n);
            t=TINV(.975,&n-1);
            b_lower= &b_est - TINV(.975,&n-1)* se_b;
            b_upper= &b_est + TINV(.975,&n-1)* se_b;
            a_lower= &a0_est - TINV(.975,&n-1)* se_a;
            a_upper= &a0_est + TINV(.975,&n-1)* se_a;
      run;

%MEND DOIT;


/*Call the %DOIT macro*/
%DOIT(example, myid, new, gold);

/*Create dataset RESULTS that stores the Deming regression estimates and CIs*/
data result;
      merge estimates variance2;
      drop _TYPE_ _FREQ_ dummy sumb suma;
      slope= STRIP(ROUND(b_est, 0.01)) || " (" ||
            STRIP(ROUND(b_lower, 0.001)) || ", " ||
            STRIP(ROUND(b_upper, 0.001)) || ")";
      int= STRIP(ROUND(a0_est, 0.01)) || " (" ||
            STRIP(ROUND(a_lower, 0.001)) || ", " ||
            STRIP(ROUND(a_upper, 0.001)) || ")";
run;

PROC SQL;
      CREATE TABLE results AS SELECT slope, int, b_est, se_b, b_lower,
      b_upper, a0_est, se_a, a_lower, a_upper
      FROM result;
QUIT;
```

Appendix 10. Concentation-exposure-duration analysis of HGVs for Phosgene (Woodall 2005). AEGL-2 value was very similar in concentration with the OEL of PEL/TLV.



Appendix 11. Calculations for conversion of mg/m^3 to ppm units

The volume of 1M of ideal gas is:

PV = nRT, since we are interested in 1M, (m/mu) = 1
PV = RT
V = RT/P

Where P = pressure (101.325 kPa)
V = volume (L)
n = 1M
R = universal gas constant (8.3144621 L·kPA/mol·K)
T = temperature (298.15K)

For 25ºC (298.15K) and 1 atm (101.325 kPa):

$V = 8.3144621 \cdot 298.15 / 101.325 = 24.4654$ L
$1\ m^3 = 1{,}000$ L

1000 L / 24.4654 L = 40.8740 M, i.e. there are 40.8740 moles of air (or any ideal gas) in 1 cubic meter ($1\ m^3$).

$1000\ ppm = 1{,}000/1{,}000{,}000 = 10^{-3} = 0.0408740\ M/m^3$
$1\ ppm = 4.08740 \cdot 10^{-5}\ M/m^3$

Therefore, assuming a standard temperature of 25ºC at 1 atm, the conversion of AEGLs in mg/m^3 to ppm is:

AEGL (ppm) = (AEGL) / ((MW/1000) · (moles of air in 1ppm)))
= AEGL [mg/m^3] / ((MW [gM]) · (1/1000 [g/mg]) · (4.08740 E-5 M/m^3) · (1/1000000))

Appendix 12. Algorithm for Prediction in Linear Regression (Davison and Hinkley 1997):

For r = 1, …., R:

1. Simulate responses y^*_r according to $Y^*_j = \hat{u}_j + \varepsilon^*_j$ j = 1, …, n,

With $\hat{u}_j = \beta_0 + \beta_1 \cdot x^*_j$ and ε^*_j is randomly sampled from $\hat{G}$

2. Obtain least squares estimates $\beta^*_j = (X^T X)^{-1} X^T) y^*_r$; then

3. For m=1,.., M,

(a) sample from $\varepsilon^*_{+,m}$ from $r1 - \bar{r}, \ldots r_n - \bar{r}$,and

(b) compute prediction error $\partial^*_{rm} = (x^T_+ \beta^*_r + \varepsilon^*_{+,m})$

The prediction interval would have limits of $\ddot{Y}_+ - a_{1-\alpha}$, $\ddot{Y}_+ - a_\alpha$,

The exact but unknown quantities are estimated by empirica; qunaitles of the pooled σ*s, whose ordered values we denote by $\sigma^*_{(1)} \leq \cdots \leq \sigma^*_{(RM)}$.

The bootstrap limits are then $\hat{y}_+ - \partial^*_{((RM+1)(1-\alpha))}$, $\hat{y}_+ - \partial^*_{((RM+1)(\alpha))}$.

Theorem 2. *The random interval* $(\overline{X} - t_{\alpha/2,n-1}\sqrt{\frac{n+1}{n}}S \ , \ \overline{X} + t_{\alpha/2,n-1}\sqrt{\frac{n+1}{n}}S)$ *is a* $100(1-\alpha)\%$*-prediction interval for* x_{n+1}.

Appendix 13. Table of existing HGVs for inhalation exposures to hazardous compounds and their respective qualitative information. These HGVs are potential sources of data for external validation of AEGLs in future analysis (Luttrell et al. 2008).

Toxicology Principles for the Industrial Hygienist

Table 27.2 — Competing Agency "Standards"

Reference Value	*Organization*	*Legal Standing*	*Type Value*	*TWA (Yes/No)*	*Exposure Duration*
PEL (Permissible Exposure Level)	OSHA	Standard	Occupational	Yes	8 hours
Ceiling	OSHA	Standard	Occupational	No	≤ 10 minutes
REL (Recommended Exposure Limit)	NIOSH	Guideline	Occupational	Yes	8 hours
IDLH (Immediately Dangerous to Life and Health)	NIOSH	Guideline	Occupational	No	≤ 10 minutes
STEL (Short Term Exposure Limit)	NIOSH	Guideline	Occupational	Yes	15 minutes
TLV (Threshold Limit Value)	ACGIH	Guideline	Occupational	Yes	8 hours
TLV-STEL (TLV Short Term Exposure Limit)	ACGIH	Guideline	Occupational	Yes	15 minutes
AEGL (Acute Exposure Guideline Level)	NAC/AEGL NAS/AEGL	Guideline	Emergency Response	Yes	10, 30 minutes and 1, 4, 8 hours
ERPG (Emergency Response Planning Guideline)	AIHA	Guideline	Emergency Response	Yes	1 hour
TEEL (Temporary Emergency Exposure Level)	DOE	Guideline	Emergency Response	Yes	1 hour
ERG (Emergency Response Guidebook)	DOT	Guideline	Emergency Response	Yes	Specialized application to determine evacuation
MRL (Minimal Risk Level)	ATSDR	Guideline	Public Health	Yes	1 – 14 days (acute) 15–364 days (intermediate) >365 days (chronic)
REL (Reference Exposure Level)	OEHHA	Guideline	Public Health	Yes	1-8 hours

Organizations: ACGIH – American Conference of Governmental Industrial Hygienists, AIHA – American Industrial Hygiene Association, ATSDR – Agency for Toxic Substances and Disease Registry, DOE – Department of Energy, DOT – Department of Transportation, NAC – National Advisory Council, NAS – National Academy of Sciences, NIOSH – National Institute for Occupational Safety and Health, OEHHA – Office of Environmental Health Hazard Assessment (California EPA), OSHA – Occupational Safety and Health Administration.

Appendix 14. Abbreviations and Terms used

AEGLs	Acute Exposure Guideline Levels
ACGIH	American Conference of Government and Industrial Hygienists
AEGL/NAC	National Advisory Committee for the Development of Acute Exposure Guideline Levels for Hazardous Substances
AIHA	American Industrial Hygiene Association
ALOHA	Areal Location of Hazardous Atmospheres
AREs	Acute reference exposures
ATSDR	Agency for Toxic Substances and Disease Registry
OSHA	Occupational Safety and Health Administration
MSHA	Mine Safety and Health Administration
BMC	Benchmark concentrations
BMC_{01}	Benchmark concentration at the lower 1% response
CAS No	Chemical Abstract Service number
DLR	Deming linear regression
DOE	The U.S. Department of Energy
DOE	The U.S. Department of Energy
ERPG	Emergency Response Planning Guideline
FACA	Federal Advisory Committee Act
LC_{50}	Lethal concentration at which 50% of experimental species die
MF	Modifying factor
mg/m^3	milligrams per cubic meter
MRLs	Minimal Risk Levels
MRLs	Minimal risk levels (ATSDR)
NAS	National Academy of Sciences
NIOSH	U.S. National Institute for Occupational Safety and Health

NOAEL	No Observed Adverse Effect Level
OEL	Occupational exposure limits
OLR	Ordinary least-squares regression
PAC	Protective Action Criteria
pHGV	provisional health guidance values
POD	point of departure
ppm	parts per million
QSAR	Quantitative Structure-Activity Relationship
RED-STEL	Recommended exposure limits - short-term exposure limit (NIOSH)
REL	California EPA's reference exposure limits
RELs	Recommended exposure limits (NIOSH)
REL-TWA	Recommended exposure limits - time-weighted average (NIOSH)
SCAPA	Subcommittee on Consequence Assessment and Protective Actions
SE	Standard error
SMILES	Simplified Molecular Input Line Entry System
SOPs	Standard Operating Procedures
TEEL	Temporary Emergency Exposure Limit
TLVs	Threshold limit values (ACGIH)
TLV-STEL	Threshold Limit Value - short-term exposure limit (ACGIH)
TLV-TWA	Threshold Limit Value - time-weighted average (ACGIH)
TSD	Technical Support Documents (AEGLs)
UF	Uncertainty factor
USEPA	US Environmental Protection Agency's

Appendix 15. Emory University's Institutional Review Board (IRB) exemption.

EMORY UNIVERSITY | Institutional Review Board

November 29, 2011

Mydung Thi Chu
RE: Determination: No IRB Review Required
IRB00054836 – AEGLs
PI: Mydung Thi Chu

Dear Mydung:

Thank you for requesting a determination from our office about the above-referenced project. Based on our review of the materials you provided, we have determined that it does not require IRB review because it does not meet the definition(s) of "research" involving "human subjects" or the definition of "clinical investigation" as set forth in Emory policies and procedures and federal rules, if applicable.

Based on the information included in the submission, you will be looking at deindentified epidemiological data that is publically available. With the end goal being to develop an efficient method that can estimate the appropriate risk level for exposure – it does not correspond with the definition of human subjects research.

This determination could be affected by substantive changes in the study design or subject population. If the project changes in any substantive way, please contact our office for clarification. Thank you for consulting the IRB

Sincerely,

Aric Edwards, BA
IRB Analyst Assistant
This letter has been digitally signed

Emory University
1599 Clifton Road, 5th Floor - Atlanta, Georgia 30322
Tel: 404.712.0720 - Fax: 404.727.1358 - Email: irb@emory.edu - Web: http://www.irb.emory.edu

Appendix 16. The Centers for Disease Control and Prevention/Agency for Toxic Substances and Disease Registry's Institutional Review Board (IRB) exemption.

Chu, Mydzung (ATSDR/DTHHS/ETB) (CTR)

From: DeCausey, Barbara (CDC/OD/OADS) on behalf of Human Subjects Review-OD (CDC)
Sent: Monday, March 19, 2012 11:07 AM
To: Chu, Mydzung (ATSDR/DTHHS/ETB) (CTR); Human Subjects Review-OD (CDC)
Cc: NCEH/ATSDR Human Subjects (CDC); Wald, Marlena (CDC/ONDIEH/NCEH)
Subject: RE: Resubmission REJECTED: Request for Review of graduate project: "Derivation of Surrogate Acute Exposure Guideline Levels (AEGLs) by Statistical Cross-Extrapolation within and across Severity Thresholds"

Hi MyDzung,

That is correct; there is no need for an IRB to review or an exemption to be requested.

Good luck with your project!
Barbara

From: Chu, Mydzung (ATSDR/DTHHS/ETB) (CTR)
Sent: Monday, March 19, 2012 10:46 AM
To: Human Subjects Review-OD (CDC)
Cc: NCEH/ATSDR Human Subjects (CDC); Wald, Marlena (CDC/ONDIEH/NCEH)
Subject: RE: Resubmission REJECTED: Request for Review of graduate project: "Derivation of Surrogate Acute Exposure Guideline Levels (AEGLs) by Statistical Cross-Extrapolation within and across Severity Thresholds"